9H-xanthene-9-carboxylic acid

Other names: 9-xanthenecarboxylic acid
Inchi: InChI=1S/C14H10O3/c15-14(16)13-9-5-1-3-7-11(9)17-12-8-4-2-6-10(12)13/h1-8,13H,(H,
InchiKey: VSBFNCXKYIEYIS-UHFFFAOYSA-N
Formula: C14H10O3
SMILES: O=C(O)C1c2ccccc2Oc2ccccc21
Mol. weight [g/mol]: 226.23

Physical Properties

Property code	Value	Unit	Source
gf	-6.45	kJ/mol	Joback Method
hf	-200.02	kJ/mol	Joback Method
hfus	33.22	kJ/mol	Joback Method
hvap	80.31	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	3.009		Crippen Method
mcvol	163.050	ml/mol	McGowan Method
pc	3547.31	kPa	Joback Method
tb	758.51	K	Joback Method
tc	990.34	K	Joback Method
tf	484.20	K	Joback Method
vc	0.615	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.77	J/mol×K	990.34	Joback Method
cpg	458.17	J/mol×K	797.15	Joback Method
cpg	468.10	J/mol×K	835.79	Joback Method
cpg	477.32	J/mol×K	874.42	Joback Method
cpg	485.94	J/mol×K	913.06	Joback Method
cpg	494.06	J/mol×K	951.70	Joback Method
cpg	447.46	J/mol×K	758.51	Joback Method
dvisc	0.0001898	Pa×s	712.79	Joback Method
dvisc	0.0002547	Pa×s	667.07	Joback Method

dvisc	0.0003568	Pa×s	621.36	Joback Method
dvisc	0.0005273	Pa×s	575.64	Joback Method
dvisc	0.0008337	Pa×s	529.92	Joback Method
dvisc	0.0001466	Pa×s	758.51	Joback Method
dvisc	0.0014372	Pa×s	484.20	Joback Method
hvapt	125.50	kJ/mol	298.15	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	1.73e-04	kPa	387.25	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	1.62e-04	kPa	387.25	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	2.17e-04	kPa	389.12	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	2.12e-04	kPa	389.12	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	2.05e-04	kPa	389.12	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	2.58e-04	kPa	391.13	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)

psub	2.45e-04	kPa	391.13	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)	
psub	3.15e-04	kPa	393.14	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)	
psub	1.35e-04	kPa	385.15	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)	
psub	3.81e-04	kPa	395.13	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)	
psub	3.78e-04	kPa	395.13	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)	
psub	3.65e-04	kPa	395.13	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)	
psub	4.81e-04	kPa	397.11	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)	

psub	4.63e-04	kPa	397.11	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)	
psub	5.60e-04	kPa	399.14	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)	
psub	5.45e-04	kPa	399.14	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)	
psub	5.52e-04	kPa	399.14	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)	
psub	6.83e-04	kPa	401.13	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)	
psub	6.94e-04	kPa	401.13	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)	
psub	6.74e-04	kPa	401.13	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)	

psub	8.36e-04	kPa	403.12	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)	
psub	8.29e-04	kPa	403.12	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)	
psub	7.82e-04	kPa	403.12	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)	
psub	9.64e-04	kPa	405.15	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)	
psub	9.41e-04	kPa	405.15	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)	
psub	1.43e-04	kPa	385.15	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)	
psub	1.48e-04	kPa	385.15	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)	

psub	1.13e-04	kPa	383.08	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	1.12e-04	kPa	383.08	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	1.19e-04	kPa	383.08	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	1.69e-04	kPa	387.25	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)
psub	3.06e-04	kPa	393.14	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2)

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Experimental and computational thermochemical studies of 9-R-xanthene derivatives (R=OH, COOH, CONH2):	https://www.doi.org/10.1016/j.jct.2012.03.017
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
psub:	Sublimation pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume