9H-Fluorene-9-carboxylic acid

Other names:	9-fluorenecarboxylic acid
	Fluorene-9-carboxylic acid
Inchi:	InChI=1S/C14H10O2/c15-14(16)13-11-7-3-1-5-9(11)10-6-2-4-8-12(10)13/h1-8,13H,(H,15
InchiKey:	DNVJGJUGFFYUPT-UHFFFAOYSA-N
Formula:	C14H10O2
SMILES:	O=C(O)C1c2ccccc2-c2ccccc21
Mol. weight [g/mol]:	210.23
CAS:	1989-33-9

Physical Properties

Property code	Value	Unit	Source
gf	91.77	kJ/mol	Joback Method
hf	-61.86	kJ/mol	Joback Method
hfus	27.34	kJ/mol	Joback Method
hvap	75.63	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	2.884		Crippen Method
mcvol	157.180	ml/mol	McGowan Method
pc	3480.65	kPa	Joback Method
rinpol	270.30		NIST Webbook
tb	727.29	K	Joback Method
tc	955.21	K	Joback Method
tf	461.15	K	Joback Method
vc	0.602	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.07	J/mol×K	727.29	Joback Method
cpg	428.82	J/mol×K	765.28	Joback Method
cpg	438.81	J/mol×K	803.26	Joback Method
cpg	448.15	J/mol×K	841.25	Joback Method
cpg	456.92	J/mol×K	879.24	Joback Method
cpg	465.25	J/mol×K	917.22	Joback Method

cpg	473.23	J/mol×K	955.21	Joback Method
dvisc	0.0011111	Pa×s	505.51	Joback Method
dvisc	0.0018279	Pa×s	461.15	Joback Method
dvisc	0.0007319	Pa×s	549.86	Joback Method
dvisc	0.0005131	Pa×s	594.22	Joback Method
dvisc	0.0003779	Pa×s	638.58	Joback Method
dvisc	0.0002896	Pa×s	682.93	Joback Method
dvisc	0.0002293	Pa×s	727.29	Joback Method
hsubt	110.10 ± 4.60	kJ/mol	383.50	NIST Webbook
rhos	1164.00	kg/m3	298.15	A combined experimental and computational thermodynamic study of fluorene-9-methanol and fluorene-9-carboxylic acid

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1989339&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
A combined experimental and computational thermodynamic study of fluorene-9-methanol and fluorene-9-carboxylic acid:	https://www.doi.org/10.1016/j.jct.2013.03.005
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure

rhos:	Solid Density
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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