

9-Fluorenone-4-carboxylic acid

Other names:	9-oxofluorene-4-carboxylic acid 9H-Fluorene-4-carboxylic acid, 9-oxo-
Inchi:	InChI=1S/C14H8O3/c15-13-9-5-2-1-4-8(9)12-10(13)6-3-7-11(12)14(16)17/h1-7H,(H,16,1
InchiKey:	AFQYQSWTVCNJQT-UHFFFAOYSA-N
Formula:	C14H8O3
SMILES:	O=C(O)c1cccc2c1-c1cccc1C2=O
Mol. weight [g/mol]:	224.22

Physical Properties

Property code	Value	Unit	Source
hf	-310.69	kJ/mol	Cheméo Relay (1.0)
hfus	25.39	kJ/mol	Joback Method
hvap	117.21	kJ/mol	Cheméo Relay (1.0)
ie	8.67	eV	Cheméo Relay (1.0)
log10ws	-3.55		Cheméo Relay (1.0)
logp	2.596		Crippen Method
mcvol	158.750	ml/mol	McGowan Method
tb	650.06	K	Cheméo Relay (1.0)
tc	999.95	K	Cheméo Relay (1.0)
tf	512.28	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	430.37	J/mol×K	804.76	Joback Method
cpg	439.96	J/mol×K	844.51	Joback Method
cpg	448.88	J/mol×K	884.26	Joback Method
cpg	457.21	J/mol×K	924.01	Joback Method
cpg	465.02	J/mol×K	963.76	Joback Method
cpg	472.41	J/mol×K	1003.50	Joback Method
cpg	479.43	J/mol×K	1043.25	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6223832&Units=SI

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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