

1-methoxyanthraquinone

Other names:	1-Methoxy-9,10-anthraquinone
Inchi:	InChI=1S/C15H10O3/c1-18-12-8-4-7-11-13(12)15(17)10-6-3-2-5-9(10)14(11)16/h2-8H,1H
InchiKey:	CQGDBBBZCJYDRY-UHFFFAOYSA-N
Formula:	C15H10O3
SMILES:	COc1cccc2c1C(=O)c1cccc1C2=O
Mol. weight [g/mol]:	238.24
CAS:	82-39-3

Physical Properties

Property code	Value	Unit	Source
gf	1.73	kJ/mol	Joback Method
hf	-222.60	kJ/mol	Joback Method
hfus	20.89	kJ/mol	Joback Method
hvap	66.48	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	2.471		Crippen Method
mcvol	172.840	ml/mol	McGowan Method
pc	2921.84	kPa	Joback Method
tb	776.10	K	Joback Method
tc	1040.20	K	Joback Method
tf	533.58	K	Joback Method
vc	0.657	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	534.36	J/molxK	996.19	Joback Method
cpg	477.07	J/molxK	776.10	Joback Method
cpg	491.04	J/molxK	820.12	Joback Method
cpg	503.74	J/molxK	864.13	Joback Method
cpg	515.19	J/molxK	908.15	Joback Method
cpg	525.39	J/molxK	952.17	Joback Method
cpg	542.10	J/molxK	1040.20	Joback Method
hsubt	106.60	kJ/mol	385.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C82393&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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