2-Methoxy-9,10-anthraquinone

Inchi: InChI=1S/C15H10O3/c1-18-9-6-7-12-13(8-9)15(17)11-5-3-2-4-10(11)14(12)16/h2-8H,1H
InchiKey: APLQXUAECQNQFE-UHFFFAOYSA-N
Formula: C15H10O3
SMILES: COc1ccc2c(c1)C(=O)c1ccccc1C2=O
Mol. weight [g/mol]: 238.24
CAS: 3274-20-2

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	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	534.36	J/mol×K	996.19	Joback Method
cpg	477.07	J/mol×K	776.10	Joback Method
cpg	491.04	J/mol×K	820.12	Joback Method
cpg	503.74	J/mol×K	864.13	Joback Method
cpg	515.19	J/mol×K	908.15	Joback Method
cpg	525.39	J/mol×K	952.17	Joback Method
cpg	542.10	J/mol×K	1040.20	Joback Method
hsubt	118.40 ± 0.40	kJ/mol	419.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3274202&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume