Anthraquinone, 1-amino-2,4-dihydroxy-

Other names: 1-amino-2,4-dihydroxyanthraquinone
Inchi: InChI=1S/C14H9NO4/c15-12-9(17)5-8(16)10-11(12)14(19)7-4-2-1-3-6(7)13(10)18/h1-5,1
InchiKey: QUXBARPXUAPKDG-UHFFFAOYSA-N
Formula: C14H9NO4
SMILES: Nc1c(O)cc(O)c2c1C(=O)c1ccccc1C2=O
Mol. weight [g/mol]: 255.23
CAS: 81-51-6

Physical Properties

Property code	Value	Unit	Source
gf	-144.48	kJ/mol	Joback Method
hf	-390.57	kJ/mol	Joback Method
hfus	33.88	kJ/mol	Joback Method
hvap	98.51	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	1.455		Crippen Method
mcvol	174.600	ml/mol	McGowan Method
pc	5235.81	kPa	Joback Method
tb	964.57	K	Joback Method
tc	1249.87	K	Joback Method
tf	806.78	K	Joback Method
vc	0.544	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	536.56	J/mol×K	964.57	Joback Method
cpg	548.97	J/mol×K	1012.12	Joback Method
cpg	561.59	J/mol×K	1059.67	Joback Method
cpg	574.62	J/mol×K	1107.22	Joback Method
cpg	588.29	J/mol×K	1154.77	Joback Method
cpg	602.82	J/mol×K	1202.32	Joback Method
cpg	618.43	J/mol×K	1249.87	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C81516&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
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