2-Amino-1-chloroanthraquinone

Inchi: InChI=1S/C14H8ClNO2/c15-12-10(16)6-5-9-11(12)14(18)8-4-2-1-3-7(8)13(9)17/h1-6H,16
InchiKey: PLGPRGMWHYWEFT-UHFFFAOYSA-N
Formula: C14H8ClNO2
SMILES: Nc1ccc2c(c1Cl)C(=O)c1ccccc1C2=O
Mol. weight [g/mol]: 257.67
CAS: 82-27-9

Physical Properties

Property code	Value	Unit	Source
gf	143.20	kJ/mol	Joback Method
hf	-63.16	kJ/mol	Joback Method
hfus	26.12	kJ/mol	Joback Method
hvap	77.53	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	2.698		Crippen Method
mcvol	175.100	ml/mol	McGowan Method
pc	3333.53	kPa	Joback Method
tb	845.74	K	Joback Method
tc	1125.67	K	Joback Method
tf	625.78	K	Joback Method
vc	0.661	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.37	J/mol×K	845.74	Joback Method
cpg	484.65	J/mol×K	892.39	Joback Method
cpg	494.74	J/mol×K	939.05	Joback Method
cpg	503.68	J/mol×K	985.70	Joback Method
cpg	511.49	J/mol×K	1032.36	Joback Method
cpg	518.22	J/mol×K	1079.01	Joback Method
cpg	523.89	J/mol×K	1125.67	Joback Method

Sources

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=C82279&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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