1-Chloro-2-methylanthraquinone

Inchi: InChI=1S/C15H9ClO2/c1-8-6-7-11-12(13(8)16)15(18)10-5-3-2-4-9(10)14(11)17/h2-7H,1H
InchiKey: NMFBXBSNLQNQKL-UHFFFAOYSA-N
Formula: C15H9ClO2
SMILES: Cc1ccc2c(c1Cl)C(=O)c1ccccc1C2=O
Mol. weight [g/mol]: 256.68
CAS: 129-35-1

Physical Properties

Property code	Value	Unit	Source
gf	85.17	kJ/mol	Joback Method
hf	-117.59	kJ/mol	Joback Method
hfus	23.51	kJ/mol	Joback Method
hvap	69.11	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	3.424		Crippen Method
mcvol	179.210	ml/mol	McGowan Method
pc	2814.34	kPa	Joback Method
tb	796.09	K	Joback Method
tc	1067.15	K	Joback Method
tf	553.79	K	Joback Method
vc	0.689	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.46	J/mol×K	796.09	Joback Method
cpg	485.43	J/mol×K	841.27	Joback Method
cpg	497.22	J/mol×K	886.44	Joback Method
cpg	507.85	J/mol×K	931.62	Joback Method
cpg	517.36	J/mol×K	976.80	Joback Method
cpg	525.77	J/mol×K	1021.97	Joback Method
cpg	533.12	J/mol×K	1067.15	Joback Method

Sources

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=C129351&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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