Anthraquinone, 2-amino-1-bromo-3-chloro-

Inchi: InChI=1S/C14H7BrClNO2/c15-11-10-8(5-9(16)12(11)17)13(18)6-3-1-2-4-7(6)14(10)19/h1
InchiKey: ZFWJIKSKKWACEX-UHFFFAOYSA-N
Formula: C14H7BrClNO2
SMILES: Nc1c(Cl)cc2c(c1Br)C(=O)c1ccccc1C2=O
Mol. weight [g/mol]: 336.57
CAS: 117-01-1

Physical Properties

Property code	Value	Unit	Source
gf	147.89	kJ/mol	Joback Method
hf	-48.30	kJ/mol	Joback Method
hfus	31.02	kJ/mol	Joback Method
hvap	84.62	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	3.460		Crippen Method
mcvol	192.600	ml/mol	McGowan Method
pc	3551.53	kPa	Joback Method
tb	916.88	K	Joback Method
tc	1205.04	K	Joback Method
tf	698.10	K	Joback Method
vc	0.724	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.48	J/mol×K	916.88	Joback Method
cpg	505.98	J/mol×K	964.91	Joback Method
cpg	514.37	J/mol×K	1012.93	Joback Method
cpg	521.71	J/mol×K	1060.96	Joback Method
cpg	528.04	J/mol×K	1108.98	Joback Method
cpg	533.39	J/mol×K	1157.01	Joback Method
cpg	537.82	J/mol×K	1205.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C117011&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