1-Amino-4-bromo-2-anthraquinone sulfonic acid

Other names: 1-amino-4-bromo-9,10-dioxoanthracene-2-sulphonic acid
Inchi: InChI=1S/C14H8BrNO5S/c15-8-5-9(22(19,20)21)12(16)11-10(8)13(17)6-3-1-2-4-7(6)14(
InchiKey: QZZSAWGVHXXMID-UHFFFAOYSA-N
Formula: C14H8BrNO5S
SMILES: Nc1c(S(=O)(=O)O)cc(Br)c2c1C(=O)c1ccccc1C2=O
Mol. weight [g/mol]: 382.19
CAS: 116-81-4

Physical Properties

Property code	Value	Unit	Source
gf	-445.54	kJ/mol	Joback Method
hf	-638.14	kJ/mol	Joback Method
hfus	42.28	kJ/mol	Joback Method
hvap	115.55	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	2.053		Crippen Method
mcvol	214.320	ml/mol	McGowan Method
pc	5146.06	kPa	Joback Method
tb	1019.41	K	Joback Method
tc	1275.42	K	Joback Method
tf	767.56	K	Joback Method
vc	0.820	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	594.71	J/mol×K	1019.41	Joback Method
cpg	600.03	J/mol×K	1062.08	Joback Method
cpg	604.04	J/mol×K	1104.75	Joback Method
cpg	606.72	J/mol×K	1147.41	Joback Method
cpg	608.09	J/mol×K	1190.08	Joback Method
cpg	608.15	J/mol×K	1232.75	Joback Method
cpg	606.90	J/mol×K	1275.42	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116814&Units=SI

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