4-Bromo-1-methylamino anthraquinone

Other names: 1-bromo-4-(methylamino)anthraquinone
Inchi: InChI=1S/C15H10BrNO2/c1-17-11-7-6-10(16)12-13(11)15(19)9-5-3-2-4-8(9)14(12)18/h2
InchiKey: IIPRUQZTMZETSL-UHFFFAOYSA-N
Formula: C15H10BrNO2
SMILES: CNc1ccc(Br)c2c1C(=O)c1ccccc1C2=O
Mol. weight [g/mol]: 316.15
CAS: 128-93-8

Physical Properties

Property code	Value	Unit	Source
gf	200.81	kJ/mol	Joback Method
hf	-22.05	kJ/mol	Joback Method
hfus	29.70	kJ/mol	Joback Method
hvap	77.60	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	3.266		Crippen Method
mcvol	194.450	ml/mol	McGowan Method
pc	3206.41	kPa	Joback Method
tb	874.99	K	Joback Method
tc	1148.06	K	Joback Method
tf	636.33	K	Joback Method
vc	0.737	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	530.18	J/mol×K	874.99	Joback Method
cpg	541.85	J/mol×K	920.50	Joback Method
cpg	552.37	J/mol×K	966.01	Joback Method
cpg	561.78	J/mol×K	1011.53	Joback Method
cpg	570.15	J/mol×K	1057.04	Joback Method
cpg	577.52	J/mol×K	1102.55	Joback Method
cpg	583.95	J/mol×K	1148.06	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=C128938&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

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