9,10-Anthracenedione, 1-amino-4-bromo-2-methyl-

Other names: Anthraquinone, 1-amino-4-bromo-2-methyl-
1-Amino-4-bromo-2-methylanthraquinone
1-Amino-2-methyl-4-bromoanthraquinone

Inchi: InChI=1S/C15H10BrNO2/c1-7-6-10(16)11-12(13(7)17)15(19)9-5-3-2-4-8(9)14(11)18/h2-6

InchiKey: VIQMJMDPUIBXQO-UHFFFAOYSA-N

Formula: C15H10BrNO2

SMILES: Cc1cc(Br)c2c(c1N)C(=O)c1ccccc1C2=O

Mol. weight [g/mol]: 316.15

CAS: 81-50-5

Physical Properties

Property code	Value	Unit	Source
gf	168.24	kJ/mol	Joback Method
hf	-53.20	kJ/mol	Joback Method
hfus	29.41	kJ/mol	Joback Method
hvap	82.47	kJ/mol	Joback Method
log10ws	-4.91		Crippen Method
logp	3.115		Crippen Method
mcvol	194.450	ml/mol	McGowan Method
pc	3314.37	kPa	Joback Method
tb	902.33	K	Joback Method
tc	1183.28	K	Joback Method
tf	679.45	K	Joback Method
vc	0.731	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	533.63	J/mol×K	902.33	Joback Method
cpg	544.77	J/mol×K	949.16	Joback Method
cpg	554.74	J/mol×K	995.98	Joback Method
cpg	563.57	J/mol×K	1042.81	Joback Method
cpg	571.32	J/mol×K	1089.63	Joback Method
cpg	578.02	J/mol×K	1136.46	Joback Method

cpg	583.71	J/mol×K	1183.28	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=C81505&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