2-Bromo-3-methylanthraquinone

Inchi: InChI=1S/C15H9BrO2/c1-8-6-11-12(7-13(8)16)15(18)10-5-3-2-4-9(10)14(11)17/h2-7H,1H
InchiKey: IXIDAURFOMZGCN-UHFFFAOYSA-N
Formula: C15H9BrO2
SMILES: Cc1cc2c(cc1Br)C(=O)c1ccccc1C2=O
Mol. weight [g/mol]: 301.13
CAS: 84-44-6

Physical Properties

Property code	Value	Unit	Source
gf	111.42	kJ/mol	Joback Method
hf	-75.52	kJ/mol	Joback Method
hfus	24.60	kJ/mol	Joback Method
hvap	71.16	kJ/mol	Joback Method
log10ws	-5.27		Crippen Method
logp	3.533		Crippen Method
mcvol	184.470	ml/mol	McGowan Method
pc	3159.72	kPa	Joback Method
tb	824.82	K	Joback Method
tc	1103.47	K	Joback Method
tf	583.67	K	Joback Method
vc	0.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	481.44	J/mol×K	824.82	Joback Method
cpg	493.94	J/mol×K	871.26	Joback Method
cpg	505.26	J/mol×K	917.70	Joback Method
cpg	515.47	J/mol×K	964.14	Joback Method
cpg	524.60	J/mol×K	1010.59	Joback Method
cpg	532.71	J/mol×K	1057.03	Joback Method
cpg	539.86	J/mol×K	1103.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C84446&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