2-Bromo-3-methylnaphthoquinone

Other names: 1,4-Naphthalenedione, 2-bromo-3-methyl-
2-Bromo-3-methyl-naphthaquinone
Inchi: InChI=1S/C11H7BrO2/c1-6-9(12)11(14)8-5-3-2-4-7(8)10(6)13/h2-5H,1H3
InchiKey: AVHXUWPFOZVLBX-UHFFFAOYSA-N
Formula: C11H7BrO2
SMILES: CC1=C(Br)C(=O)c2ccccc2C1=O
Mol. weight [g/mol]: 251.08
CAS: 3129-39-3

Physical Properties

Property code	Value	Unit	Source
gf	-19.28	kJ/mol	Joback Method
hf	-172.56	kJ/mol	Joback Method
hfus	17.61	kJ/mol	Joback Method
hvap	59.96	kJ/mol	Joback Method
ie	9.25	eV	NIST Webbook
ie	9.63 ± 0.01	eV	NIST Webbook
log10ws	-3.89		Crippen Method
logp	2.735		Crippen Method
mcvol	147.570	ml/mol	McGowan Method
pc	3786.98	kPa	Joback Method
tb	709.34	K	Joback Method
tc	982.80	K	Joback Method
tf	493.37	K	Joback Method
vc	0.555	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.51	J/mol×K	709.34	Joback Method
cpg	360.99	J/mol×K	754.92	Joback Method
cpg	372.43	J/mol×K	800.49	Joback Method
cpg	382.83	J/mol×K	846.07	Joback Method
cpg	392.17	J/mol×K	891.64	Joback Method

cpg	400.44	J/mol×K	937.22	Joback Method
cpg	407.64	J/mol×K	982.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3129393&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
ie:	Ionization energy
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