Naphthalene, 1-bromo-5-nitro-

Other names: 1-Bromo-5-nitronaphthalene
5-Bromo-1-nitronaphthalene
Inchi: InChI=1S/C10H6BrNO2/c11-9-5-1-4-8-7(9)3-2-6-10(8)12(13)14/h1-6H
InchiKey: OTYRDQXZRJZHOX-UHFFFAOYSA-N
Formula: C10H6BrNO2
SMILES: O=[N+]([O-])c1cccc2c(Br)cccc12
Mol. weight [g/mol]: 252.06
CAS: 5328-76-7

Physical Properties

Property code	Value	Unit	Source
gf	282.99	kJ/mol	Joback Method
hf	170.50	kJ/mol	Joback Method
hfus	28.58	kJ/mol	Joback Method
hvap	66.12	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	3.510		Crippen Method
mcvol	143.460	ml/mol	McGowan Method
pc	4156.97	kPa	Joback Method
tb	701.82	K	Joback Method
tc	981.59	K	Joback Method
tf	490.03	K	Joback Method
vc	0.553	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.04	J/mol×K	701.82	Joback Method
cpg	334.00	J/mol×K	748.45	Joback Method
cpg	343.05	J/mol×K	795.08	Joback Method
cpg	351.29	J/mol×K	841.71	Joback Method
cpg	358.88	J/mol×K	888.33	Joback Method
cpg	365.94	J/mol×K	934.96	Joback Method
cpg	372.60	J/mol×K	981.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5328767&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