Phenol, 2,6-dibromo-4-nitro-

Other names: 2,6-Dibromo-4-nitrophenol
4-Nitro-2,6-dibromophenol
Inchi: InChI=1S/C6H3Br2NO3/c7-4-1-3(9(11)12)2-5(8)6(4)10/h1-2,10H
InchiKey: WBHYZUAQCSHXCT-UHFFFAOYSA-N
Formula: C6H3Br2NO3
SMILES: O=[N+]([O-])c1cc(Br)c(O)c(Br)c1
Mol. weight [g/mol]: 296.90
CAS: 99-28-5

Physical Properties

Property code	Value	Unit	Source
gf	2.36	kJ/mol	Joback Method
hf	-88.99	kJ/mol	Joback Method
hfus	32.27	kJ/mol	Joback Method
hvap	75.03	kJ/mol	Joback Method
log10ws	-4.00		Crippen Method
logp	2.825		Crippen Method
mcvol	129.930	ml/mol	McGowan Method
pc	7014.41	kPa	Joback Method
tb	738.10	K	Joback Method
tc	1028.23	K	Joback Method
tf	583.77	K	Joback Method
vc	0.435	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	260.74	J/mol×K	738.10	Joback Method
cpg	266.63	J/mol×K	786.46	Joback Method
cpg	272.19	J/mol×K	834.81	Joback Method
cpg	277.59	J/mol×K	883.17	Joback Method
cpg	283.01	J/mol×K	931.52	Joback Method
cpg	288.63	J/mol×K	979.88	Joback Method
cpg	294.60	J/mol×K	1028.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C99285&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

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