Benzene, 1,2-dibromo-4-nitro-

Inchi: InChI=1S/C6H3Br2NO2/c7-5-2-1-4(9(10)11)3-6(5)8/h1-3H
InchiKey: DLLDRYLYVHKDKK-UHFFFAOYSA-N
Formula: C6H3Br2NO2
SMILES: O=[N+]([O-])c1ccc(Br)c(Br)c1
Mol. weight [g/mol]: 280.90
CAS: 5411-50-7

Physical Properties

Property code	Value	Unit	Source
gf	156.98	kJ/mol	Joback Method
hf	88.32	kJ/mol	Joback Method
hfus	26.49	kJ/mol	Joback Method
hvap	62.01	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	3.120		Crippen Method
mcvol	124.060	ml/mol	McGowan Method
pc	5544.32	kPa	Joback Method
tb	569.20	K	NIST Webbook
tc	941.96	K	Joback Method
tf	472.05	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	229.96	J/mol×K	657.48	Joback Method
cpg	237.11	J/mol×K	704.89	Joback Method
cpg	243.55	J/mol×K	752.31	Joback Method
cpg	249.34	J/mol×K	799.72	Joback Method
cpg	254.59	J/mol×K	847.14	Joback Method
cpg	259.35	J/mol×K	894.55	Joback Method
cpg	263.72	J/mol×K	941.96	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	453.20	K	2.70	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5411507&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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