Benzene, 2-bromo-1,3,5-trinitro-

Other names: 2-bromo-1,3,5-trinitrobenzene
Inchi: InChI=1S/C6H2BrN3O6/c7-6-4(9(13)14)1-3(8(11)12)2-5(6)10(15)16/h1-2H
InchiKey: WJAMDVPZHYCFJH-UHFFFAOYSA-N
Formula: C6H2BrN3O6
SMILES: O=[N+]([O-])c1cc([N+](=O)[O-])c(Br)c([N+](=O)[O-])c1
Mol. weight [g/mol]: 292.00
CAS: 4185-53-9

Physical Properties

Property code	Value	Unit	Source
gf	204.13	kJ/mol	Joback Method
hf	29.00	kJ/mol	Joback Method
hfus	43.54	kJ/mol	Joback Method
hvap	89.42	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	2.174		Crippen Method
mcvol	141.400	ml/mol	McGowan Method
pc	5080.25	kPa	Joback Method
tb	899.98	K	Joback Method
tc	1205.04	K	Joback Method
tf	711.99	K	Joback Method
vc	0.572	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.86	J/mol×K	899.98	Joback Method
cpg	344.36	J/mol×K	950.82	Joback Method
cpg	349.14	J/mol×K	1001.67	Joback Method
cpg	353.26	J/mol×K	1052.51	Joback Method
cpg	356.82	J/mol×K	1103.35	Joback Method
cpg	359.89	J/mol×K	1154.20	Joback Method
cpg	362.57	J/mol×K	1205.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4185539&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