

Benzene, 1-bromo-2,4-dinitro-

Other names:	1-Bromo-2,4-dinitrobenzene 2,4-Dinitrobromobenzene 4-Bromo-1,3-dinitrobenzene o,p-Dinitrophenyl bromide 2,4-Dinitrophenyl bromide
Inchi:	InChI=1S/C6H3BrN2O4/c7-5-2-1-4(8(10)11)3-6(5)9(12)13/h1-3H
InchiKey:	PBOPJYORIDJAFE-UHFFFAOYSA-N
Formula:	C6H3BrN2O4
SMILES:	O=[N+]([O-])c1ccc(Br)c([N+](=O)[O-])c1
Mol. weight [g/mol]:	247.00
CAS:	584-48-5

Physical Properties

Property code	Value	Unit	Source
gf	178.21	kJ/mol	Joback Method
hf	51.23	kJ/mol	Joback Method
hfus	32.57	kJ/mol	Joback Method
hvap	72.17	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	2.265		Crippen Method
mcvol	123.980	ml/mol	McGowan Method
pc	5102.04	kPa	Joback Method
rinpol	1755.00		NIST Webbook
rinpol	1755.00		NIST Webbook
tb	743.16	K	Joback Method
tc	1035.01	K	Joback Method
tf	555.86	K	Joback Method
vc	0.489	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.37	J/molxK	743.16	Joback Method
cpg	282.66	J/molxK	791.80	Joback Method

cpg	289.14	J/mol×K	840.44	Joback Method
cpg	294.92	J/mol×K	889.09	Joback Method
cpg	300.05	J/mol×K	937.73	Joback Method
cpg	304.61	J/mol×K	986.37	Joback Method
cpg	308.69	J/mol×K	1035.01	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C584485&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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