Methane, bromotrinitro-

Other names:	Bromotrinitromethane
	Bromopicrin
Inchi:	InChI=1S/CBrN3O6/c2-1(3(6)7,4(8)9)5(10)11
InchiKey:	KWSSHZBBUQSMKF-UHFFFAOYSA-N
Formula:	CBrN3O6
SMILES:	O=[N+]([O-])C(Br)([N+](=O)[O-])[N+](=O)[O-]
Mol. weight [g/mol]:	229.93
CAS:	560-95-2

Physical Properties

Property code	Value	Unit	Source
gf	81.35	kJ/mol	Joback Method
hf	94.60	kJ/mol	NIST Webbook
hfl	48.50	kJ/mol	NIST Webbook
hfl	13.50 ± 1.00	kJ/mol	NIST Webbook
hfus	30.30	kJ/mol	Joback Method
hvap	46.00	kJ/mol	NIST Webbook
hvap	47.74	kJ/mol	NIST Webbook
log10ws	-2.52		Crippen Method
logp	-0.177		Crippen Method
mcvol	94.710	ml/mol	McGowan Method
pc	7061.65	kPa	Joback Method
tb	740.73	K	Joback Method
tc	1047.74	K	Joback Method
tf	594.08	K	Joback Method
vc	0.389	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	205.86	J/mol×K	740.73	Joback Method
cpg	209.62	J/mol×K	791.90	Joback Method
cpg	212.78	J/mol×K	843.07	Joback Method
cpg	215.48	J/mol×K	894.23	Joback Method

cpg	217.84	J/mol×K	945.40	Joback Method
cpg	220.01	J/mol×K	996.57	Joback Method
cpg	222.11	J/mol×K	1047.74	Joback Method
hvapt	47.80	kJ/mol	326.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C560952&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
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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