

trinitromethane

Inchi: InChI=1S/CHN3O6/c5-2(6)1(3(7)8)4(9)10/h1H
InchiKey: LZGVDNRJCGPNDS-UHFFFAOYSA-N
Formula: CHN3O6
SMILES: O=[N+](O-)C([N+](=O)[O-])[N+](=O)[O-]
Mol. weight [g/mol]: 151.04
CAS: 517-25-9

Physical Properties

Property code	Value	Unit	Source
chl	-504.30	kJ/mol	NIST Webbook
chl	-458.48	kJ/mol	NIST Webbook
chs	-520.90	kJ/mol	NIST Webbook
chs	-488.00 ± 13.00	kJ/mol	NIST Webbook
gf	61.75	kJ/mol	Joback Method
hf	-101.53	kJ/mol	Joback Method
hfl	-77.95	kJ/mol	NIST Webbook
hfl	-32.10	kJ/mol	NIST Webbook
hfl	-68.00 ± 3.10	kJ/mol	NIST Webbook
hfs	-48.00 ± 2.00	kJ/mol	NIST Webbook
hfus	28.91	kJ/mol	Joback Method
hsub	45.20 ± 2.10	kJ/mol	NIST Webbook
hsub	46.00 ± 0.42	kJ/mol	NIST Webbook
hvap	54.80	kJ/mol	NIST Webbook
ie	12.23	eV	NIST Webbook
log10ws	-1.60		Crippen Method
logp	-0.900		Crippen Method
mcvol	77.210	ml/mol	McGowan Method
pc	6200.01	kPa	Joback Method
tb	677.36	K	Joback Method
tc	961.37	K	Joback Method
tf	292.00 ± 3.00	K	NIST Webbook
vc	0.332	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	184.70	J/mol×K	677.36	Joback Method
cpg	190.07	J/mol×K	724.69	Joback Method
cpg	194.82	J/mol×K	772.03	Joback Method
cpg	198.98	J/mol×K	819.36	Joback Method
cpg	202.60	J/mol×K	866.70	Joback Method
cpg	205.70	J/mol×K	914.03	Joback Method
cpg	208.33	J/mol×K	961.37	Joback Method
hvapt	32.60	kJ/mol	303.50	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C517259&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

chl:	Standard liquid enthalpy of combustion
chs:	Standard solid enthalpy of combustion
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
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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

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