

Methane, iodotrinitro-

Other names:	Iodotrinitromethane
Inchi:	InChI=1S/CIN3O6/c2-1(3(6)7,4(8)9)5(10)11
InchiKey:	PVYWOZWHSJHJFC-UHFFFAOYSA-N
Formula:	CIN3O6
SMILES:	O=[N+](O-)C(I)([N+](=O)[O-])[N+](=O)[O-]
Mol. weight [g/mol]:	276.93
CAS:	630-70-6

Physical Properties

Property code	Value	Unit	Source
gf	125.15	kJ/mol	Joback Method
hf	163.00	kJ/mol	NIST Webbook
hfs	114.00	kJ/mol	NIST Webbook
hfus	29.42	kJ/mol	Joback Method
hsub	49.00	kJ/mol	NIST Webbook
hvap	75.67	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	-0.137		Crippen Method
mcpvol	103.030	ml/mol	McGowan Method
pc	6093.99	kPa	Joback Method
tb	767.71	K	Joback Method
tc	1092.62	K	Joback Method
tf	592.34	K	Joback Method
vc	0.414	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	208.77	J/molxK	767.71	Joback Method
cpg	212.16	J/molxK	821.86	Joback Method
cpg	214.99	J/molxK	876.01	Joback Method
cpg	217.43	J/molxK	930.17	Joback Method
cpg	219.63	J/molxK	984.32	Joback Method
cpg	221.77	J/molxK	1038.47	Joback Method

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=C630706&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
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
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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