Methyldinitramine

Inchi: InChI=1S/CH3N3O4/c1-2(3(5)6)4(7)8/h1H3
InchiKey: AAIWMHUUYNFKAM-UHFFFAOYSA-N
Formula: CH3N3O4
SMILES: CN([N+](=O)[O-])[N+](=O)[O-]
Mol. weight [g/mol]: 121.05
CAS: 25346-05-8

Physical Properties

Property code	Value	Unit	Source
chs	-823.80 ± 0.70	kJ/mol	NIST Webbook
gf	139.42	kJ/mol	Joback Method
hf	53.50 ± 0.80	kJ/mol	NIST Webbook
hf	43.10 ± 6.30	kJ/mol	NIST Webbook
hfl	1.70 ± 0.80	kJ/mol	NIST Webbook
hfs	1.50 ± 0.70	kJ/mol	NIST Webbook
hfus	24.09	kJ/mol	Joback Method
hsub	52.00 ± 0.40	kJ/mol	NIST Webbook
hvap	41.40 ± 5.40	kJ/mol	NIST Webbook
log10ws	-0.96		Crippen Method
logp	-0.698		Crippen Method
mcvol	69.770	ml/mol	McGowan Method
pc	5990.66	kPa	Joback Method
tb	538.40	K	Joback Method
tc	786.86	K	Joback Method
tf	420.72	K	Joback Method
vc	0.274	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	154.34	J/mol×K	538.40	Joback Method
cpg	160.92	J/mol×K	579.81	Joback Method
cpg	166.93	J/mol×K	621.22	Joback Method
cpg	172.41	J/mol×K	662.63	Joback Method

cpg	177.39	J/mol×K	704.04	Joback Method
cpg	181.91	J/mol×K	745.45	Joback Method
cpg	185.99	J/mol×K	786.86	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=C25346058&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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
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