N,N'-Dimethyl-N,N'-dinitrourea

Inchi: InChI=1S/C3H6N4O5/c1-4(6(9)10)3(8)5(2)7(11)12/h1-2H3
InchiKey: FEQAJOCLTADZKX-UHFFFAOYSA-N
Formula: C3H6N4O5
SMILES: CN(C(=O)N(C)[N+](=O)[O-])[N+](=O)[O-]
Mol. weight [g/mol]: 178.10
CAS: 25466-50-6

Physical Properties

Property code	Value	Unit	Source
chl	-1928.60	kJ/mol	NIST Webbook
gf	138.12	kJ/mol	Joback Method
hf	-104.29	kJ/mol	Joback Method
hfl	-109.50	kJ/mol	NIST Webbook
hfus	33.89	kJ/mol	Joback Method
hvap	66.29	kJ/mol	Joback Method
log10ws	-1.12		Crippen Method
logp	-0.647		Crippen Method
mcvol	109.500	ml/mol	McGowan Method
pc	4938.44	kPa	Joback Method
tb	650.47	K	Joback Method
tc	891.39	K	Joback Method
tf	525.66	K	Joback Method
vc	0.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	280.28	J/mol×K	650.47	Joback Method
cpg	288.65	J/mol×K	690.62	Joback Method
cpg	296.26	J/mol×K	730.78	Joback Method
cpg	303.17	J/mol×K	770.93	Joback Method
cpg	309.43	J/mol×K	811.09	Joback Method
cpg	315.09	J/mol×K	851.24	Joback Method
cpg	320.20	J/mol×K	891.39	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=C25466506&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid 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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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