1,1-Dinitropropane

Inchi: InChI=1S/C3H6N2O4/c1-2-3(4(6)7)5(8)9/h3H,2H2,1H3
InchiKey: DFHLCCWFLMSKJI-UHFFFAOYSA-N
Formula: C3H6N2O4
SMILES: CCC([N+](=O)[O-])[N+](=O)[O-]
Mol. weight [g/mol]: 134.09
CAS: 601-76-3

Physical Properties

Property code	Value	Unit	Source
chl	-1875.00 ± 1.00	kJ/mol	NIST Webbook
chl	-1867.40 ± 1.40	kJ/mol	NIST Webbook
gf	43.04	kJ/mol	Joback Method
hf	-132.05	kJ/mol	Joback Method
hfl	-163.00 ± 1.00	kJ/mol	NIST Webbook
hfl	-170.60 ± 1.40	kJ/mol	NIST Webbook
hfus	22.73	kJ/mol	Joback Method
hvap	62.47 ± 0.63	kJ/mol	NIST Webbook
log10ws	-1.85		Crippen Method
logp	0.276		Crippen Method
mcvol	87.970	ml/mol	McGowan Method
pc	4602.62	kPa	Joback Method
tb	571.28	K	Joback Method
tc	819.28	K	Joback Method
tf	395.79	K	Joback Method
vc	0.361	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	205.50	J/mol×K	571.28	Joback Method
cpg	214.01	J/mol×K	612.61	Joback Method
cpg	221.89	J/mol×K	653.95	Joback Method
cpg	229.18	J/mol×K	695.28	Joback Method
cpg	235.90	J/mol×K	736.61	Joback Method

cpg	242.08	J/mol×K	777.94	Joback Method
cpg	247.74	J/mol×K	819.28	Joback Method
hvapt	57.90	kJ/mol	353.00	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C601763&Units=SI&Mask=3FFF

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
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