

1,3-Dinitropropane

Inchi:	InChI=1S/C3H6N2O4/c6-4(7)2-1-3-5(8)9/h1-3H2
InchiKey:	ITUGOFFBEXBDGZ-UHFFFAOYSA-N
Formula:	C3H6N2O4
SMILES:	O=[N+]([O-])CCC[N+](=O)[O-]
Mol. weight [g/mol]:	134.09
CAS:	6125-21-9

Physical Properties

Property code	Value	Unit	Source
chl	-1831.00 ± 0.80	kJ/mol	NIST Webbook
chl	-1814.10 ± 1.40	kJ/mol	NIST Webbook
gf	45.48	kJ/mol	Joback Method
hf	-126.77	kJ/mol	Joback Method
hfl	-223.90 ± 1.40	kJ/mol	NIST Webbook
hfl	-207.00 ± 0.80	kJ/mol	NIST Webbook
hfus	26.25	kJ/mol	Joback Method
hvap	55.45	kJ/mol	Joback Method
log10ws	-1.25		Crippen Method
logp	-0.070		Crippen Method
mcvol	87.970	ml/mol	McGowan Method
pc	4553.06	kPa	Joback Method
tb	571.72	K	Joback Method
tc	814.08	K	Joback Method
tf	251.80 ± 0.10	K	NIST Webbook
vc	0.367	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	205.03	J/mol×K	571.72	Joback Method
cpg	213.28	J/mol×K	612.11	Joback Method
cpg	220.95	J/mol×K	652.51	Joback Method
cpg	228.06	J/mol×K	692.90	Joback Method
cpg	234.64	J/mol×K	733.29	Joback Method

cpg	240.71	J/mol×K	773.68	Joback Method
cpg	246.31	J/mol×K	814.08	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C6125219&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
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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