2,2-Dinitropropane

Inchi: InChI=1S/C3H6N2O4/c1-3(2,4(6)7)5(8)9/h1-2H3
InchiKey: DHPRWWYQIUXCQM-UHFFFAOYSA-N
Formula: C3H6N2O4
SMILES: CC(C)([N+](=O)[O-])[N+](=O)[O-]
Mol. weight [g/mol]: 134.09
CAS: 595-49-3

Physical Properties

Property code	Value	Unit	Source
chs	-1846.00 ± 1.00	kJ/mol	NIST Webbook
chs	-1850.30 ± 2.70	kJ/mol	NIST Webbook
gf	48.32	kJ/mol	Joback Method
hf	-135.52	kJ/mol	Joback Method
hfs	-192.00 ± 1.00	kJ/mol	NIST Webbook
hfs	-187.70 ± 2.70	kJ/mol	NIST Webbook
hfus	18.83	kJ/mol	Joback Method
hvap	54.16	kJ/mol	Joback Method
log10ws	-1.85		Crippen Method
logp	0.276		Crippen Method
mcvol	87.970	ml/mol	McGowan Method
pc	4672.09	kPa	Joback Method
tb	458.70	K	NIST Webbook
tb	326.05	K	KDB
tc	827.42	K	Joback Method
tf	326.00 ± 1.00	K	NIST Webbook
tt	324.50 ± 0.20	K	NIST Webbook
vc	0.356	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	209.10	J/mol×K	568.49	Joback Method
cpg	217.87	J/mol×K	611.65	Joback Method
cpg	225.82	J/mol×K	654.80	Joback Method

cpg	233.03	J/mol×K	697.96	Joback Method
cpg	239.55	J/mol×K	741.11	Joback Method
cpg	245.46	J/mol×K	784.27	Joback Method
cpg	250.81	J/mol×K	827.42	Joback Method
cps	205.00	J/mol×K	300.00	NIST Webbook
cps	206.30	J/mol×K	298.00	NIST Webbook
hfust	2.64	kJ/mol	324.50	NIST Webbook
hfust	11.28	kJ/mol	267.70	NIST Webbook
hfust	1.87	kJ/mol	259.70	NIST Webbook
hfust	2.64	kJ/mol	324.50	NIST Webbook
hvapt	46.30	kJ/mol	458.00	NIST Webbook
sfust	42.13	J/mol×K	267.70	NIST Webbook
sfust	7.20	J/mol×K	259.70	NIST Webbook
sfust	8.12	J/mol×K	324.50	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C595493&Units=SI&Mask=3FFF
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
KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1430
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
cps: Solid phase 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
hfust: Enthalpy of fusion at a given temperature
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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume