

Propane, 2-chloro-2-nitro-

Other names:	2-Chloro-2-nitropropane
Inchi:	InChI=1S/C3H6ClNO2/c1-3(2,4)5(6)7/h1-2H3
InchiKey:	JQYFSFNSNVRUPY-UHFFFAOYSA-N
Formula:	C3H6ClNO2
SMILES:	CC(C)(Cl)[N+](=O)[O-]
Mol. weight [g/mol]:	123.54
CAS:	594-71-8

Physical Properties

Property code	Value	Unit	Source
gf	0.84	kJ/mol	Joback Method
hf	-140.50	kJ/mol	Joback Method
hfus	11.67	kJ/mol	Joback Method
hvap	41.95	kJ/mol	Joback Method
log10ws	-1.92		Crippen Method
logp	1.238		Crippen Method
mcvol	82.790	ml/mol	McGowan Method
pc	4374.18	kPa	Joback Method
tb	454.08	K	Joback Method
tc	685.88	K	Joback Method
tf	251.60 ± 0.10	K	NIST Webbook
vc	0.324	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	157.74	J/mol×K	454.08	Joback Method
cpg	166.12	J/mol×K	492.71	Joback Method
cpg	173.82	J/mol×K	531.35	Joback Method
cpg	180.90	J/mol×K	569.98	Joback Method
cpg	187.39	J/mol×K	608.61	Joback Method
cpg	193.34	J/mol×K	647.24	Joback Method
cpg	198.80	J/mol×K	685.88	Joback Method
hfust	1.34	kJ/mol	261.60	NIST Webbook

hfust	9.54	kJ/mol	213.80	NIST Webbook
hfust	1.34	kJ/mol	261.60	NIST Webbook
sfust	44.62	J/mol×K	213.80	NIST Webbook
sfust	5.10	J/mol×K	261.60	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C594718&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	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
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
vc:	Critical Volume

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