

Ethyl 2-nitropropionate

Other names:	Propanoic acid, 2-nitro-, ethyl ester Propionic acid, 2-nitro-, ethyl ester
Inchi:	InChI=1S/C5H9NO4/c1-3-10-5(7)4(2)6(8)9/h4H,3H2,1-2H3
InchiKey:	ZXBGJDZWJJFFQY-UHFFFAOYSA-N
Formula:	C5H9NO4
SMILES:	CCOC(=O)C(C)[N+](=O)[O-]
Mol. weight [g/mol]:	147.13
CAS:	2531-80-8

Physical Properties

Property code	Value	Unit	Source
gf	-209.59	kJ/mol	Joback Method
hf	-407.37	kJ/mol	Joback Method
hfus	19.33	kJ/mol	Joback Method
hvap	52.08	kJ/mol	Joback Method
log10ws	-0.97		Crippen Method
logp	0.215		Crippen Method
mvol	106.170	ml/mol	McGowan Method
pc	3754.57	kPa	Joback Method
tb	463.70	K	NIST Webbook
tc	758.30	K	Joback Method
tf	346.88	K	Joback Method
vc	0.415	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.84	J/molxK	541.49	Joback Method
cpg	253.68	J/molxK	577.62	Joback Method
cpg	263.02	J/molxK	613.76	Joback Method
cpg	271.86	J/molxK	649.89	Joback Method
cpg	280.19	J/molxK	686.03	Joback Method
cpg	288.03	J/molxK	722.16	Joback Method
cpg	295.35	J/molxK	758.30	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	348.70	K	1.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2531808&Units=SI
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

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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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