1-Nitro-2-propanol

Other names: 2-Propanol, 1-nitro-
Inchi: InChI=1S/C3H7NO3/c1-3(5)2-4(6)7/h3,5H,2H2,1H3
InchiKey: PFNCKQIYLAVYJF-UHFFFAOYSA-N
Formula: C3H7NO3
SMILES: CC(O)C[N+](=O)[O-]
Mol. weight [g/mol]: 105.09
CAS: 3156-73-8

Physical Properties

Property code	Value	Unit	Source
gf	-129.33	kJ/mol	Joback Method
hf	-273.52	kJ/mol	Joback Method
hfus	15.45	kJ/mol	Joback Method
hvap	55.15	kJ/mol	Joback Method
log10ws	-0.54		Crippen Method
logp	-0.356		Crippen Method
mcvol	76.420	ml/mol	McGowan Method
pc	5146.06	kPa	Joback Method
tb	511.62	K	Joback Method
tc	713.17	K	Joback Method
tf	313.00	K	Joback Method
vc	0.298	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	169.65	J/mol×K	511.62	Joback Method
cpg	176.61	J/mol×K	545.21	Joback Method
cpg	183.21	J/mol×K	578.80	Joback Method
cpg	189.44	J/mol×K	612.39	Joback Method
cpg	195.33	J/mol×K	645.98	Joback Method
cpg	200.89	J/mol×K	679.58	Joback Method
cpg	206.13	J/mol×K	713.17	Joback Method

Sources

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=C3156738&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume