1-Propanol, 2,2-dimethyl-, nitrate

Other names: Neopentyl nitrate
2,2-Dimethyl-1-propyl nitrate
Inchi: InChI=1S/C5H11NO3/c1-5(2,3)4-9-6(7)8/h4H2,1-3H3
InchiKey: YJGBGWFCCCQXIM-UHFFFAOYSA-N
Formula: C5H11NO3
SMILES: CC(C)(C)CO[N+](=O)[O-]
Mol. weight [g/mol]: 133.15
CAS: 926-42-1

Physical Properties

Property code	Value	Unit	Source
gf	-75.39	kJ/mol	Joback Method
hf	-298.26	kJ/mol	Joback Method
hfus	13.84	kJ/mol	Joback Method
hvap	44.43	kJ/mol	Joback Method
log10ws	-1.84		Crippen Method
logp	1.241		Crippen Method
mcvol	104.600	ml/mol	McGowan Method
pc	3526.27	kPa	Joback Method
tb	484.83	K	Joback Method
tc	701.21	K	Joback Method
tf	314.37	K	Joback Method
vc	0.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.20	J/mol×K	484.83	Joback Method
cpg	245.59	J/mol×K	520.89	Joback Method
cpg	256.32	J/mol×K	556.96	Joback Method
cpg	266.41	J/mol×K	593.02	Joback Method
cpg	275.89	J/mol×K	629.08	Joback Method
cpg	284.78	J/mol×K	665.15	Joback Method
cpg	293.10	J/mol×K	701.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C926421&Units=SI
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

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