3-Pentyl nitrate

Inchi: InChI=1S/C5H11NO3/c1-3-5(4-2)9-6(7)8/h5H,3-4H2,1-2H3
InchiKey: WQZKKVJFBZPJSU-UHFFFAOYSA-N
Formula: C5H11NO3
SMILES: CCC(CC)O[N+](=O)[O-]
Mol. weight [g/mol]: 133.15

Physical Properties

Property code	Value	Unit	Source
gf	-80.67	kJ/mol	Joback Method
hf	-294.79	kJ/mol	Joback Method
hfus	17.73	kJ/mol	Joback Method
hvap	45.34	kJ/mol	Joback Method
log10ws	-2.19		Crippen Method
logp	1.383		Crippen Method
mcvol	104.600	ml/mol	McGowan Method
pc	3480.65	kPa	Joback Method
rinpol	844.00		NIST Webbook
rinpol	844.00		NIST Webbook
tb	487.62	K	Joback Method
tc	695.13	K	Joback Method
tf	296.95	K	Joback Method
vc	0.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.11	J/mol×K	487.62	Joback Method
cpg	241.83	J/mol×K	522.21	Joback Method
cpg	252.06	J/mol×K	556.79	Joback Method
cpg	261.83	J/mol×K	591.38	Joback Method
cpg	271.12	J/mol×K	625.96	Joback Method
cpg	279.95	J/mol×K	660.55	Joback Method
cpg	288.32	J/mol×K	695.13	Joback Method

Sources

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=R496952&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume