2-Methyl-3-hexyl nitrate

Inchi: InChI=1S/C7H15NO3/c1-4-5-7(6(2)3)11-8(9)10/h6-7H,4-5H2,1-3H3
InchiKey: LCSOOXWRLLYSSV-UHFFFAOYSA-N
Formula: C7H15NO3
SMILES: CCCC(O[N+](=O)[O-])C(C)C
Mol. weight [g/mol]: 161.20

Physical Properties

Property code	Value	Unit	Source
gf	-66.27	kJ/mol	Joback Method
hf	-341.35	kJ/mol	Joback Method
hfus	19.39	kJ/mol	Joback Method
hvap	49.40	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	2.019		Crippen Method
mcvol	132.780	ml/mol	McGowan Method
pc	2832.35	kPa	Joback Method
rinpol	996.00		NIST Webbook
tb	532.94	K	Joback Method
tc	738.90	K	Joback Method
tf	304.49	K	Joback Method
vc	0.515	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	317.68	J/mol×K	532.94	Joback Method
cpg	330.92	J/mol×K	567.27	Joback Method
cpg	343.52	J/mol×K	601.59	Joback Method
cpg	355.50	J/mol×K	635.92	Joback Method
cpg	366.86	J/mol×K	670.25	Joback Method
cpg	377.61	J/mol×K	704.57	Joback Method
cpg	387.77	J/mol×K	738.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R496794&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume