3-Hexyl nitrate

Inchi: InChI=1S/C6H13NO3/c1-3-5-6(4-2)10-7(8)9/h6H,3-5H2,1-2H3
InchiKey: OJOZCOXRANAOPV-UHFFFAOYSA-N
Formula: C6H13NO3
SMILES: CCCC(CC)O[N+](=O)[O-]
Mol. weight [g/mol]: 147.17

Physical Properties

Property code	Value	Unit	Source
gf	-72.25	kJ/mol	Joback Method
hf	-315.43	kJ/mol	Joback Method
hfus	20.32	kJ/mol	Joback Method
hvap	47.56	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	1.773		Crippen Method
mcvol	118.690	ml/mol	McGowan Method
pc	3117.52	kPa	Joback Method
rinpol	935.00		NIST Webbook
rinpol	935.00		NIST Webbook
tb	510.50	K	Joback Method
tc	715.03	K	Joback Method
tf	308.22	K	Joback Method
vc	0.466	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.25	J/mol×K	510.50	Joback Method
cpg	285.12	J/mol×K	544.59	Joback Method
cpg	296.45	J/mol×K	578.68	Joback Method
cpg	307.25	J/mol×K	612.76	Joback Method
cpg	317.51	J/mol×K	646.85	Joback Method
cpg	327.26	J/mol×K	680.94	Joback Method
cpg	336.48	J/mol×K	715.03	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R496907&Units=SI

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