3-Methyl-2-pentyl nitrate, diastereomer # 1

Inchi: InChI=1S/C6H13NO3/c1-4-5(2)6(3)10-7(8)9/h5-6H,4H2,1-3H3/t5-,6+/m1/s1
InchiKey: IEHIEWLLOPOHIZ-RITPCOANSA-N
Formula: C6H13NO3
SMILES: CCC(C)C(C)O[N+](=O)[O-]
Mol. weight [g/mol]: 147.17

Physical Properties

Property code	Value	Unit	Source
gf	-74.69	kJ/mol	Joback Method
hf	-320.71	kJ/mol	Joback Method
hfus	16.80	kJ/mol	Joback Method
hvap	47.17	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	1.629		Crippen Method
mcvol	118.690	ml/mol	McGowan Method
pc	3145.56	kPa	Joback Method
rinpol	927.00		NIST Webbook
tb	510.06	K	Joback Method
tc	719.18	K	Joback Method
tf	293.22	K	Joback Method
vc	0.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.53	J/mol×K	510.06	Joback Method
cpg	285.74	J/mol×K	544.91	Joback Method
cpg	297.38	J/mol×K	579.77	Joback Method
cpg	308.45	J/mol×K	614.62	Joback Method
cpg	318.96	J/mol×K	649.47	Joback Method
cpg	328.91	J/mol×K	684.33	Joback Method
cpg	338.30	J/mol×K	719.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R496927&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