4-Methyl-3-heptyl nitrate, diastereomer # 1

Inchi: InChI=1S/C8H17NO3/c1-4-6-7(3)8(5-2)12-9(10)11/h7-8H,4-6H2,1-3H3/t7-,8+/m1/s1
InchiKey: GIQRQCALXYZGQY-SFYZADRCSA-N
Formula: C8H17NO3
SMILES: CCCC(C)C(CC)O[N+](=O)[O-]
Mol. weight [g/mol]: 175.23

Physical Properties

Property code	Value	Unit	Source
gf	-57.85	kJ/mol	Joback Method
hf	-361.99	kJ/mol	Joback Method
hfus	21.98	kJ/mol	Joback Method
hvap	51.63	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	2.410		Crippen Method
mcvol	146.870	ml/mol	McGowan Method
pc	2563.69	kPa	Joback Method
rinpol	1093.00		NIST Webbook
rinpol	1093.00		NIST Webbook
rinpol	1093.00		NIST Webbook
tb	555.82	K	Joback Method
tc	758.71	K	Joback Method
tf	315.76	K	Joback Method
vc	0.572	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	363.71	J/mol×K	555.82	Joback Method
cpg	377.84	J/mol×K	589.63	Joback Method
cpg	391.28	J/mol×K	623.45	Joback Method
cpg	404.05	J/mol×K	657.26	Joback Method
cpg	416.15	J/mol×K	691.08	Joback Method
cpg	427.60	J/mol×K	724.89	Joback Method
cpg	438.40	J/mol×K	758.71	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R496605&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