2-Ethyl-1-hexyl nitrate

Inchi: InChI=1S/C8H17NO3/c1-3-5-6-8(4-2)7-12-9(10)11/h8H,3-7H2,1-2H3
InchiKey: NKRVGWFEFKCZAP-UHFFFAOYSA-N
Formula: C8H17NO3
SMILES: CCCCC(CC)CO[N+](=O)[O-]
Mol. weight [g/mol]: 175.23

Physical Properties

Property code	Value	Unit	Source
gf	-55.41	kJ/mol	Joback Method
hf	-356.71	kJ/mol	Joback Method
hfus	25.50	kJ/mol	Joback Method
hvap	52.02	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	2.411		Crippen Method
mcvol	146.870	ml/mol	McGowan Method
pc	2543.05	kPa	Joback Method
rinpol	1145.00		NIST Webbook
rinpol	1145.00		NIST Webbook
tb	556.26	K	Joback Method
tc	754.99	K	Joback Method
tf	330.76	K	Joback Method
vc	0.578	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	363.36	J/mol×K	556.26	Joback Method
cpg	377.14	J/mol×K	589.38	Joback Method
cpg	390.27	J/mol×K	622.50	Joback Method
cpg	402.76	J/mol×K	655.63	Joback Method
cpg	414.62	J/mol×K	688.75	Joback Method
cpg	425.87	J/mol×K	721.87	Joback Method
cpg	436.50	J/mol×K	754.99	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=R496561&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