6-Undecyl nitrate

Inchi: InChI=1S/C11H23NO3/c1-3-5-7-9-11(15-12(13)14)10-8-6-4-2/h11H,3-10H2,1-2H3
InchiKey: QKIRWTVGFDYQDE-UHFFFAOYSA-N
Formula: C11H23NO3
SMILES: CCCCCC(CCCCC)O[N+](=O)[O-]
Mol. weight [g/mol]: 217.31

Physical Properties

Property code	Value	Unit	Source
gf	-30.15	kJ/mol	Joback Method
hf	-418.63	kJ/mol	Joback Method
hfus	33.27	kJ/mol	Joback Method
hvap	58.69	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	3.724		Crippen Method
mcvol	189.140	ml/mol	McGowan Method
pc	1938.95	kPa	Joback Method
rinpol	1411.00		NIST Webbook
tb	624.90	K	Joback Method
tc	816.18	K	Joback Method
tf	364.57	K	Joback Method
vc	0.746	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	511.55	J/mol×K	624.90	Joback Method
cpg	527.36	J/mol×K	656.78	Joback Method
cpg	542.39	J/mol×K	688.66	Joback Method
cpg	556.68	J/mol×K	720.54	Joback Method
cpg	570.22	J/mol×K	752.42	Joback Method
cpg	583.05	J/mol×K	784.30	Joback Method
cpg	595.16	J/mol×K	816.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R497024&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

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