2-Tetradecyl nitrate

Inchi: InChI=1S/C14H29NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14(2)18-15(16)17/h14H,3-13H2,1-2
InchiKey: ZHCKWOJTMJJKCR-UHFFFAOYSA-N
Formula: C14H29NO3
SMILES: CCCCCCCCCCCCC(C)O[N+](=O)[O-]
Mol. weight [g/mol]: 259.38

Physical Properties

Property code	Value	Unit	Source
gf	-4.89	kJ/mol	Joback Method
hf	-480.55	kJ/mol	Joback Method
hfus	41.04	kJ/mol	Joback Method
hvap	65.37	kJ/mol	Joback Method
log10ws	-5.96		Crippen Method
logp	4.894		Crippen Method
mcvol	231.410	ml/mol	McGowan Method
pc	1527.07	kPa	Joback Method
rinpol	1756.00		NIST Webbook
tb	693.54	K	Joback Method
tc	880.04	K	Joback Method
tf	398.38	K	Joback Method
vc	0.913	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	672.97	J/mol×K	693.54	Joback Method
cpg	690.13	J/mol×K	724.62	Joback Method
cpg	706.43	J/mol×K	755.71	Joback Method
cpg	721.89	J/mol×K	786.79	Joback Method
cpg	736.52	J/mol×K	817.87	Joback Method
cpg	750.35	J/mol×K	848.96	Joback Method
cpg	763.40	J/mol×K	880.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R496878&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

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