1-Tetradecyl nitrate

Inchi: InChI=1S/C14H29NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-18-15(16)17/h2-14H2,1H3
InchiKey: DUNXOJJZJRNHEK-UHFFFAOYSA-N
Formula: C14H29NO3
SMILES: CCCCCCCCCCCCCCO[N+](=O)[O-]
Mol. weight [g/mol]: 259.38

Physical Properties

Property code	Value	Unit	Source
gf	-2.45	kJ/mol	Joback Method
hf	-475.27	kJ/mol	Joback Method
hfus	44.57	kJ/mol	Joback Method
hvap	65.76	kJ/mol	Joback Method
log10ws	-5.84		Crippen Method
logp	4.896		Crippen Method
mcvol	231.410	ml/mol	McGowan Method
pc	1517.57	kPa	Joback Method
rinpol	1819.00		NIST Webbook
tb	693.98	K	Joback Method
tc	877.90	K	Joback Method
tf	413.38	K	Joback Method
vc	0.919	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	672.50	J/mol×K	693.98	Joback Method
cpg	689.40	J/mol×K	724.63	Joback Method
cpg	705.47	J/mol×K	755.29	Joback Method
cpg	720.72	J/mol×K	785.94	Joback Method
cpg	735.19	J/mol×K	816.60	Joback Method
cpg	748.88	J/mol×K	847.25	Joback Method
cpg	761.82	J/mol×K	877.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R496690&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