1-Pentadecyl nitrate

Inchi: InChI=1S/C15H31NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-19-16(17)18/h2-15H2,1H3
InchiKey: YIEWNNIDJUKTQV-UHFFFAOYSA-N
Formula: C15H31NO3
SMILES: CCCCCCCCCCCCCCCO[N+](=O)[O-]
Mol. weight [g/mol]: 273.41

Physical Properties

Property code	Value	Unit	Source
gf	5.97	kJ/mol	Joback Method
hf	-495.91	kJ/mol	Joback Method
hfus	47.15	kJ/mol	Joback Method
hvap	67.98	kJ/mol	Joback Method
log10ws	-6.26		Crippen Method
logp	5.286		Crippen Method
mcvol	245.500	ml/mol	McGowan Method
pc	1410.13	kPa	Joback Method
rinpol	1920.00		NIST Webbook
rinpol	1920.00		NIST Webbook
tb	716.86	K	Joback Method
tc	900.27	K	Joback Method
tf	424.65	K	Joback Method
vc	0.976	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	728.82	J/mol×K	716.86	Joback Method
cpg	746.10	J/mol×K	747.43	Joback Method
cpg	762.52	J/mol×K	778.00	Joback Method
cpg	778.10	J/mol×K	808.57	Joback Method
cpg	792.86	J/mol×K	839.13	Joback Method
cpg	806.82	J/mol×K	869.70	Joback Method
cpg	820.01	J/mol×K	900.27	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=R496685&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