2-Pentadecyl nitrate

Inchi: InChI=1S/C15H31NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15(2)19-16(17)18/h15H,3-14H2
InchiKey: XOJWQOCAZSZVPN-UHFFFAOYSA-N
Formula: C15H31NO3
SMILES: CCCCCCCCCCCCCC(C)O[N+](=O)[O-]
Mol. weight [g/mol]: 273.41

Physical Properties

Property code	Value	Unit	Source
gf	3.53	kJ/mol	Joback Method
hf	-501.19	kJ/mol	Joback Method
hfus	43.63	kJ/mol	Joback Method
hvap	67.60	kJ/mol	Joback Method
log10ws	-6.37		Crippen Method
logp	5.284		Crippen Method
mcvol	245.500	ml/mol	McGowan Method
pc	1418.64	kPa	Joback Method
rinpol	1857.00		NIST Webbook
tb	716.42	K	Joback Method
tc	902.15	K	Joback Method
tf	409.65	K	Joback Method
vc	0.970	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	729.30	J/mol×K	716.42	Joback Method
cpg	746.82	J/mol×K	747.37	Joback Method
cpg	763.45	J/mol×K	778.33	Joback Method
cpg	779.21	J/mol×K	809.28	Joback Method
cpg	794.12	J/mol×K	840.24	Joback Method
cpg	808.20	J/mol×K	871.19	Joback Method
cpg	821.48	J/mol×K	902.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R496858&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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