Undecyl nitrate

Inchi: InChI=1S/C11H23NO3/c1-2-3-4-5-6-7-8-9-10-11-15-12(13)14/h2-11H2,1H3
InchiKey: VTALQOYOTZKULH-UHFFFAOYSA-N
Formula: C11H23NO3
SMILES: CCCCCCCCCCCO[N+](=O)[O-]
Mol. weight [g/mol]: 217.31

Physical Properties

Property code	Value	Unit	Source
gf	-27.71	kJ/mol	Joback Method
hf	-413.35	kJ/mol	Joback Method
hfus	36.79	kJ/mol	Joback Method
hvap	59.08	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	3.725		Crippen Method
mcvol	189.140	ml/mol	McGowan Method
pc	1925.36	kPa	Joback Method
rinpol	1513.00		NIST Webbook
rinpol	1513.00		NIST Webbook
tb	625.34	K	Joback Method
tc	813.30	K	Joback Method
tf	379.57	K	Joback Method
vc	0.751	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	511.12	J/mol×K	625.34	Joback Method
cpg	526.62	J/mol×K	656.67	Joback Method
cpg	541.37	J/mol×K	687.99	Joback Method
cpg	555.41	J/mol×K	719.32	Joback Method
cpg	568.74	J/mol×K	750.65	Joback Method
cpg	581.38	J/mol×K	781.98	Joback Method
cpg	593.35	J/mol×K	813.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R497059&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