

Tridecyl nitrate

Inchi:	InChI=1S/C13H27NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-17-14(15)16/h2-13H2,1H3
InchiKey:	DMUORYXPGSLKKV-UHFFFAOYSA-N
Formula:	C13H27NO3
SMILES:	CCCCCCCCCCCCCO[N+](=O)[O-]
Mol. weight [g/mol]:	245.36

Physical Properties

Property code	Value	Unit	Source
gf	-10.87	kJ/mol	Joback Method
hf	-454.63	kJ/mol	Joback Method
hfus	41.98	kJ/mol	Joback Method
hvap	63.53	kJ/mol	Joback Method
log10ws	-5.43		Crippen Method
logp	4.506		Crippen Method
mcvol	217.320	ml/mol	McGowan Method
pc	1637.78	kPa	Joback Method
rinpol	1717.00		NIST Webbook
tb	671.10	K	Joback Method
tc	855.99	K	Joback Method
tf	402.11	K	Joback Method
vc	0.864	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	617.39	J/molxK	671.10	Joback Method
cpg	633.87	J/molxK	701.91	Joback Method
cpg	649.55	J/molxK	732.73	Joback Method
cpg	664.45	J/molxK	763.54	Joback Method
cpg	678.58	J/molxK	794.36	Joback Method
cpg	691.97	J/molxK	825.17	Joback Method
cpg	704.63	J/molxK	855.99	Joback Method

Sources

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=R497044&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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