2-Dodecyl nitrate

Inchi: InChI=1S/C12H25NO3/c1-3-4-5-6-7-8-9-10-11-12(2)16-13(14)15/h12H,3-11H2,1-2H3
InchiKey: TZINGABWMPNNOT-UHFFFAOYSA-N
Formula: C12H25NO3
SMILES: CCCCCCCCCCC(C)O[N+](=O)[O-]
Mol. weight [g/mol]: 231.33

Physical Properties

Property code	Value	Unit	Source
gf	-21.73	kJ/mol	Joback Method
hf	-439.27	kJ/mol	Joback Method
hfus	35.86	kJ/mol	Joback Method
hvap	60.92	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	4.114		Crippen Method
mcvol	203.230	ml/mol	McGowan Method
pc	1784.86	kPa	Joback Method
rinpol	1554.00		NIST Webbook
tb	647.78	K	Joback Method
tc	837.11	K	Joback Method
tf	375.84	K	Joback Method
vc	0.801	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	564.01	J/mol×K	647.78	Joback Method
cpg	580.33	J/mol×K	679.33	Joback Method
cpg	595.84	J/mol×K	710.89	Joback Method
cpg	610.57	J/mol×K	742.44	Joback Method
cpg	624.53	J/mol×K	774.00	Joback Method
cpg	637.74	J/mol×K	805.55	Joback Method
cpg	650.22	J/mol×K	837.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R496749&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