

Dodecyl nitrate

Inchi:	InChI=1S/C12H25NO3/c1-2-3-4-5-6-7-8-9-10-11-12-16-13(14)15/h2-12H2,1H3
InchiKey:	PAWHIGFHUHHWLN-UHFFFAOYSA-N
Formula:	C12H25NO3
SMILES:	CCCCCCCCCCCCO[N+](=O)[O-]
Mol. weight [g/mol]:	231.33
CAS:	13277-59-3

Physical Properties

Property code	Value	Unit	Source
gf	-19.29	kJ/mol	Joback Method
hf	-433.99	kJ/mol	Joback Method
hfus	39.38	kJ/mol	Joback Method
hvap	61.31	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	4.116		Crippen Method
mvol	203.230	ml/mol	McGowan Method
pc	1772.85	kPa	Joback Method
rinpol	1615.00		NIST Webbook
rinpol	1615.00		NIST Webbook
tb	648.22	K	Joback Method
tc	834.47	K	Joback Method
tf	390.84	K	Joback Method
vc	0.807	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	563.57	J/molxK	648.22	Joback Method
cpg	579.58	J/molxK	679.26	Joback Method
cpg	594.83	J/molxK	710.30	Joback Method
cpg	609.32	J/molxK	741.34	Joback Method
cpg	623.08	J/molxK	772.39	Joback Method
cpg	636.12	J/molxK	803.43	Joback Method
cpg	648.46	J/molxK	834.47	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=C13277593&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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