

Hydratropic acid, nonyl ester

Inchi:	InChI=1S/C18H28O2/c1-3-4-5-6-7-8-12-15-20-18(19)16(2)17-13-10-9-11-14-17/h9-11,13
InchiKey:	LPCSAZLTDVQCPI-UHFFFAOYSA-N
Formula:	C18H28O2
SMILES:	CCCCCCCCCOC(=O)C(C)c1cccc1
Mol. weight [g/mol]:	276.41

Physical Properties

Property code	Value	Unit	Source
gf	-23.27	kJ/mol	Joback Method
hf	-428.40	kJ/mol	Joback Method
hfus	35.68	kJ/mol	Joback Method
hvap	66.71	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	5.084		Crippen Method
mcvol	248.160	ml/mol	McGowan Method
pc	1524.69	kPa	Joback Method
rinpol	2491.00		NIST Webbook
rinpol	2491.00		NIST Webbook
tb	713.77	K	Joback Method
tc	908.55	K	Joback Method
tf	376.20	K	Joback Method
vc	0.954	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	711.39	J/molxK	713.77	Joback Method
cpg	791.65	J/molxK	876.08	Joback Method
cpg	777.54	J/molxK	843.62	Joback Method
cpg	762.49	J/molxK	811.16	Joback Method
cpg	746.47	J/molxK	778.70	Joback Method
cpg	729.45	J/molxK	746.23	Joback Method
cpg	804.86	J/molxK	908.55	Joback Method
dvisc	0.0000886	Paxs	713.77	Joback Method

dvisc	0.0001187	Paxs	657.51	Joback Method
dvisc	0.0001681	Paxs	601.25	Joback Method
dvisc	0.0002558	Paxs	544.99	Joback Method
dvisc	0.0004288	Paxs	488.72	Joback Method
dvisc	0.0008220	Paxs	432.46	Joback Method
dvisc	0.0019145	Paxs	376.20	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=U415066&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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

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