

Hydratropic acid, hexadecyl ester

Inchi:	InChI=1S/C25H42O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-19-22-27-25(26)23(2)24-20-17
InchiKey:	OJOVCGNNBABGAZ-UHFFFAOYSA-N
Formula:	C25H42O2
SMILES:	CCCCCCCCCCCCCCCCOC(=O)C(C)c1ccccc1
Mol. weight [g/mol]:	374.60

Physical Properties

Property code	Value	Unit	Source
gf	35.67	kJ/mol	Joback Method
hf	-572.88	kJ/mol	Joback Method
hfus	53.81	kJ/mol	Joback Method
hvap	82.29	kJ/mol	Joback Method
log10ws	-8.22		Crippen Method
logp	7.815		Crippen Method
mcvol	346.790	ml/mol	McGowan Method
pc	956.73	kPa	Joback Method
rinsol	2032.00		NIST Webbook
tb	873.93	K	Joback Method
tc	1072.51	K	Joback Method
tf	455.09	K	Joback Method
vc	1.345	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1130.30	J/molxK	873.93	Joback Method
cpg	1149.94	J/molxK	907.03	Joback Method
cpg	1168.34	J/molxK	940.12	Joback Method
cpg	1185.55	J/molxK	973.22	Joback Method
cpg	1201.62	J/molxK	1006.32	Joback Method
cpg	1216.61	J/molxK	1039.42	Joback Method
cpg	1230.57	J/molxK	1072.51	Joback Method
dvisc	0.0008889	Paxs	455.09	Joback Method
dvisc	0.0003588	Paxs	524.90	Joback Method

dvisc	0.0001792	Paxs	594.70	Joback Method
dvisc	0.0001036	Paxs	664.51	Joback Method
dvisc	0.0000664	Paxs	734.32	Joback Method
dvisc	0.0000460	Paxs	804.12	Joback Method
dvisc	0.0000338	Paxs	873.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415073&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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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