Hydratropic acid, hexyl ester

Inchi: InChI=1S/C15H22O2/c1-3-4-5-9-12-17-15(16)13(2)14-10-7-6-8-11-14/h6-8,10-11,13H,3-
InchiKey: LARAVRJCBZOBAA-UHFFFAOYSA-N
Formula: C15H22O2
SMILES: CCCCCCOC(=O)C(C)c1ccccc1
Mol. weight [g/mol]: 234.33

Physical Properties

Property code	Value	Unit	Source
gf	-48.53	kJ/mol	Joback Method
hf	-366.48	kJ/mol	Joback Method
hfus	27.91	kJ/mol	Joback Method
hvap	60.03	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	3.914		Crippen Method
mcvol	205.890	ml/mol	McGowan Method
pc	1935.54	kPa	Joback Method
rinpol	2176.00		NIST Webbook
rinpol	2176.00		NIST Webbook
tb	645.13	K	Joback Method
tc	846.21	K	Joback Method
tf	342.39	K	Joback Method
vc	0.785	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	546.83	J/mol×K	645.13	Joback Method
cpg	563.95	J/mol×K	678.64	Joback Method
cpg	580.10	J/mol×K	712.16	Joback Method
cpg	595.30	J/mol×K	745.67	Joback Method
cpg	609.57	J/mol×K	779.18	Joback Method
cpg	622.96	J/mol×K	812.70	Joback Method
cpg	635.49	J/mol×K	846.21	Joback Method
dvisc	0.0024547	Pa×s	342.39	Joback Method

dvisc	0.0010907	Pa×s	392.85	Joback Method
dvisc	0.0005830	Pa×s	443.30	Joback Method
dvisc	0.0003541	Pa×s	493.76	Joback Method
dvisc	0.0002360	Pa×s	544.22	Joback Method
dvisc	0.0001684	Pa×s	594.67	Joback Method
dvisc	0.0001267	Pa×s	645.13	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=U415063&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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