Hydratropic acid, undecyl ester

Inchi: InChI=1S/C20H32O2/c1-3-4-5-6-7-8-9-10-14-17-22-20(21)18(2)19-15-12-11-13-16-19/h1
InchiKey: GKFILJMPFQBUIF-UHFFFAOYSA-N
Formula: C20H32O2
SMILES: CCCCCCCCCCCOC(=O)C(C)c1ccccc1
Mol. weight [g/mol]: 304.47

Physical Properties

Property code	Value	Unit	Source
gf	-6.43	kJ/mol	Joback Method
hf	-469.68	kJ/mol	Joback Method
hfus	40.86	kJ/mol	Joback Method
hvap	71.16	kJ/mol	Joback Method
log10ws	-6.12		Crippen Method
logp	5.864		Crippen Method
mcvol	276.340	ml/mol	McGowan Method
pc	1319.43	kPa	Joback Method
rinpol	2702.00		NIST Webbook
rinpol	2702.00		NIST Webbook
tb	759.53	K	Joback Method
tc	952.34	K	Joback Method
tf	398.74	K	Joback Method
vc	1.065	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	826.70	J/mol×K	759.53	Joback Method
cpg	845.21	J/mol×K	791.66	Joback Method
cpg	862.64	J/mol×K	823.80	Joback Method
cpg	879.02	J/mol×K	855.93	Joback Method
cpg	894.41	J/mol×K	888.07	Joback Method
cpg	908.82	J/mol×K	920.20	Joback Method
cpg	922.31	J/mol×K	952.34	Joback Method
dvisc	0.0015731	Pa×s	398.74	Joback Method

dvisc	0.0006621	Pa×s	458.87	Joback Method
dvisc	0.0003406	Pa×s	519.00	Joback Method
dvisc	0.0002011	Pa×s	579.13	Joback Method
dvisc	0.0001311	Pa×s	639.27	Joback Method
dvisc	0.0000920	Pa×s	699.40	Joback Method
dvisc	0.0000683	Pa×s	759.53	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415068&Units=SI

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