Hydratropic acid, oct-3-en-2-yl ester

Inchi: InChI=1S/C17H24O2/c1-4-5-6-8-11-14(2)19-17(18)15(3)16-12-9-7-10-13-16/h7-15H,4-6
InchiKey: WWWYXJRNGBBOCF-DHZHZOJOSA-N
Formula: C17H24O2
SMILES: CCCCC=CC(C)OC(=O)C(C)c1ccccc1
Mol. weight [g/mol]: 260.37

Physical Properties

Property code	Value	Unit	Source
gf	46.09	kJ/mol	Joback Method
hf	-295.82	kJ/mol	Joback Method
hfus	29.77	kJ/mol	Joback Method
hvap	64.05	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	4.468		Crippen Method
mcvol	229.770	ml/mol	McGowan Method
pc	1728.90	kPa	Joback Method
rinpol	1743.00		NIST Webbook
rinpol	1743.00		NIST Webbook
tb	694.61	K	Joback Method
tc	901.31	K	Joback Method
tf	344.85	K	Joback Method
vc	0.872	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	633.29	J/mol×K	694.61	Joback Method
cpg	650.94	J/mol×K	729.06	Joback Method
cpg	667.51	J/mol×K	763.51	Joback Method
cpg	683.04	J/mol×K	797.96	Joback Method
cpg	697.59	J/mol×K	832.41	Joback Method
cpg	711.20	J/mol×K	866.86	Joback Method
cpg	723.92	J/mol×K	901.31	Joback Method
dvisc	0.0025274	Pa×s	344.85	Joback Method

dvisc	0.0009377	Pa×s	403.14	Joback Method
dvisc	0.0004469	Pa×s	461.44	Joback Method
dvisc	0.0002515	Pa×s	519.73	Joback Method
dvisc	0.0001590	Pa×s	578.02	Joback Method
dvisc	0.0001093	Pa×s	636.32	Joback Method
dvisc	0.0000800	Pa×s	694.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406957&Units=SI
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

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