Hydratropic acid, 3-methylbut-2-en-1-yl ester

Inchi: InChI=1S/C14H18O2/c1-11(2)9-10-16-14(15)12(3)13-7-5-4-6-8-13/h4-9,12H,10H2,1-3H3
InchiKey: KLOHAVOEOBEPHC-UHFFFAOYSA-N
Formula: C14H18O2
SMILES: CC(C)=CCOC(=O)C(C)c1ccccc1
Mol. weight [g/mol]: 218.29

Physical Properties

Property code	Value	Unit	Source
gf	14.72	kJ/mol	Joback Method
hf	-238.41	kJ/mol	Joback Method
hfus	24.21	kJ/mol	Joback Method
hvap	57.84	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.299		Crippen Method
mcvol	187.500	ml/mol	McGowan Method
pc	2224.99	kPa	Joback Method
rinpol	1573.00		NIST Webbook
rinpol	1573.00		NIST Webbook
tb	626.29	K	Joback Method
tc	842.02	K	Joback Method
tf	312.08	K	Joback Method
vc	0.711	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.50	J/mol×K	626.29	Joback Method
cpg	489.94	J/mol×K	662.24	Joback Method
cpg	505.35	J/mol×K	698.20	Joback Method
cpg	519.77	J/mol×K	734.15	Joback Method
cpg	533.25	J/mol×K	770.11	Joback Method
cpg	545.84	J/mol×K	806.06	Joback Method
cpg	557.57	J/mol×K	842.02	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=U406955&Units=SI

Legend

cpg:	Ideal gas heat capacity
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