Isochavicol 2-methylbutyrate

Inchi: InChI=1S/C14H18O2/c1-4-6-12-7-9-13(10-8-12)16-14(15)11(3)5-2/h4,6-11H,5H2,1-3H3
InchiKey: QVAWDXCSFUFEAT-UHFFFAOYSA-N
Formula: C14H18O2
SMILES: CC=Cc1ccc(OC(=O)C(C)CC)cc1
Mol. weight [g/mol]: 218.29

Physical Properties

Property code	Value	Unit	Source
gf	13.64	kJ/mol	Joback Method
hf	-240.09	kJ/mol	Joback Method
hfus	25.13	kJ/mol	Joback Method
hvap	58.42	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	3.671		Crippen Method
mcvol	187.500	ml/mol	McGowan Method
pc	2183.60	kPa	Joback Method
rinpol	1654.00		NIST Webbook
rinpol	1651.00		NIST Webbook
rinpol	1651.00		NIST Webbook
rinpol	1654.00		NIST Webbook
rinpol	1648.00		NIST Webbook
rinpol	1651.00		NIST Webbook
ripol	2255.00		NIST Webbook
ripol	2256.00		NIST Webbook
ripol	2256.00		NIST Webbook
tb	631.39	K	Joback Method
tc	844.45	K	Joback Method
tf	338.56	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.31	J/mol×K	631.39	Joback Method

cpg	543.99	J/mol×K	808.94	Joback Method
cpg	531.62	J/mol×K	773.43	Joback Method
cpg	518.41	J/mol×K	737.92	Joback Method
cpg	504.31	J/mol×K	702.41	Joback Method
cpg	489.29	J/mol×K	666.90	Joback Method
cpg	555.54	J/mol×K	844.45	Joback Method
dvisc	0.0001195	Pa×s	631.39	Joback Method
dvisc	0.0001557	Pa×s	582.59	Joback Method
dvisc	0.0002128	Pa×s	533.78	Joback Method
dvisc	0.0003099	Pa×s	484.98	Joback Method
dvisc	0.0004908	Pa×s	436.17	Joback Method
dvisc	0.0008729	Pa×s	387.37	Joback Method
dvisc	0.0018328	Pa×s	338.56	Joback Method

Sources

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=R614165&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume