Isochavicol isobutyrate

Inchi: InChI=1S/C13H16O2/c1-4-5-11-6-8-12(9-7-11)15-13(14)10(2)3/h4-10H,1-3H3
InchiKey: LJEWVBGJLXRKQV-UHFFFAOYSA-N
Formula: C13H16O2
SMILES: CC=Cc1ccc(OC(=O)C(C)C)cc1
Mol. weight [g/mol]: 204.26

Physical Properties

Property code	Value	Unit	Source
gf	5.22	kJ/mol	Joback Method
hf	-219.45	kJ/mol	Joback Method
hfus	22.54	kJ/mol	Joback Method
hvap	56.20	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	3.281		Crippen Method
mcvol	173.410	ml/mol	McGowan Method
pc	2393.53	kPa	Joback Method
rinpol	1538.00		NIST Webbook
rinpol	1546.00		NIST Webbook
rinpol	1541.00		NIST Webbook
rinpol	1538.00		NIST Webbook
rinpol	1541.00		NIST Webbook
rinpol	1541.00		NIST Webbook
ripol	2134.00		NIST Webbook
ripol	2136.00		NIST Webbook
ripol	2136.00		NIST Webbook
tb	608.51	K	Joback Method
tc	825.22	K	Joback Method
tf	327.29	K	Joback Method
vc	0.653	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	423.05	J/mol×K	608.51	Joback Method

cpg	491.15	J/mol×K	789.10	Joback Method
cpg	479.26	J/mol×K	752.98	Joback Method
cpg	466.54	J/mol×K	716.86	Joback Method
cpg	452.95	J/mol×K	680.75	Joback Method
cpg	438.47	J/mol×K	644.63	Joback Method
cpg	502.25	J/mol×K	825.22	Joback Method
dvisc	0.0001316	Pa×s	608.51	Joback Method
dvisc	0.0001707	Pa×s	561.64	Joback Method
dvisc	0.0002323	Pa×s	514.77	Joback Method
dvisc	0.0003361	Pa×s	467.90	Joback Method
dvisc	0.0005281	Pa×s	421.03	Joback Method
dvisc	0.0009292	Pa×s	374.16	Joback Method
dvisc	0.0019222	Pa×s	327.29	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=R614150&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

ripol: Polar retention indices

tb: Normal Boiling Point Temperature

tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume