

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	1541.00		NIST Webbook
rinpol	1546.00		NIST Webbook
rinpol	1538.00		NIST Webbook
rinpol	1541.00		NIST Webbook
rinpol	1541.00		NIST Webbook
rinpol	1538.00		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/molxK	608.51	Joback Method

cpg	438.47	J/molxK	644.63	Joback Method
cpg	452.95	J/molxK	680.75	Joback Method
cpg	466.54	J/molxK	716.86	Joback Method
cpg	479.26	J/molxK	752.98	Joback Method
cpg	491.15	J/molxK	789.10	Joback Method
cpg	502.25	J/molxK	825.22	Joback Method
dvisc	0.0019222	Paxs	327.29	Joback Method
dvisc	0.0009292	Paxs	374.16	Joback Method
dvisc	0.0005281	Paxs	421.03	Joback Method
dvisc	0.0003361	Paxs	467.90	Joback Method
dvisc	0.0002323	Paxs	514.77	Joback Method
dvisc	0.0001707	Paxs	561.64	Joback Method
dvisc	0.0001316	Paxs	608.51	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=R614150&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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