6-Methoxythymol isobutyrate

Inchi: InChI=1S/C15H22O3/c1-6-7-13(16)18-15-12(10(2)3)9-8-11(4)14(15)17-5/h8-10H,6-7H2,
InchiKey: OVEFHMXINPFAGU-UHFFFAOYSA-N
Formula: C15H22O3
SMILES: CCCC(=O)Oc1c(C(C)C)ccc(C)c1OC
Mol. weight [g/mol]: 250.33

Physical Properties

Property code	Value	Unit	Source
gf	-182.42	kJ/mol	Joback Method
hf	-533.11	kJ/mol	Joback Method
hfus	27.93	kJ/mol	Joback Method
hvap	64.42	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	3.833		Crippen Method
mcvol	211.760	ml/mol	McGowan Method
pc	1834.11	kPa	Joback Method
rinpol	1671.00		NIST Webbook
tb	682.49	K	Joback Method
tc	884.50	K	Joback Method
tf	402.18	K	Joback Method
vc	0.803	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.55	J/mol×K	682.49	Joback Method
cpg	589.82	J/mol×K	716.16	Joback Method
cpg	605.22	J/mol×K	749.83	Joback Method
cpg	619.74	J/mol×K	783.50	Joback Method
cpg	633.37	J/mol×K	817.17	Joback Method
cpg	646.14	J/mol×K	850.84	Joback Method
cpg	658.02	J/mol×K	884.50	Joback Method
dvisc	0.0008542	Pa×s	402.18	Joback Method
dvisc	0.0004921	Pa×s	448.90	Joback Method

dvisc	0.0003146	Pa×s	495.62	Joback Method
dvisc	0.0002172	Pa×s	542.34	Joback Method
dvisc	0.0001591	Pa×s	589.05	Joback Method
dvisc	0.0001220	Pa×s	635.77	Joback Method
dvisc	0.0000970	Pa×s	682.49	Joback Method

Sources

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=R226976&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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