

2-(Isobutyryloxy)-thymol methyl ether

Inchi:	InChI=1S/C15H22O3/c1-9(2)12-8-7-11(5)13(14(12)17-6)18-15(16)10(3)4/h7-10H,1-6H3
InchiKey:	RIOPMYZNXSYRON-UHFFFAOYSA-N
Formula:	C15H22O3
SMILES:	COc1c(C(C)C)ccc(C)c1OC(=O)C(C)C
Mol. weight [g/mol]:	250.33

Physical Properties

Property code	Value	Unit	Source
gf	-184.86	kJ/mol	Joback Method
hf	-538.39	kJ/mol	Joback Method
hfus	24.41	kJ/mol	Joback Method
hvap	64.04	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	3.688		Crippen Method
mcvol	211.760	ml/mol	McGowan Method
pc	1846.75	kPa	Joback Method
rinsol	1675.00		NIST Webbook
tb	682.05	K	Joback Method
tc	887.57	K	Joback Method
tf	387.18	K	Joback Method
vc	0.797	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.04	J/molxK	682.05	Joback Method
cpg	590.62	J/molxK	716.30	Joback Method
cpg	606.29	J/molxK	750.56	Joback Method
cpg	621.03	J/molxK	784.81	Joback Method
cpg	634.86	J/molxK	819.06	Joback Method
cpg	647.77	J/molxK	853.31	Joback Method
cpg	659.76	J/molxK	887.57	Joback Method
dvisc	0.0010114	Paxs	387.18	Joback Method
dvisc	0.0005382	Paxs	436.32	Joback Method

dvisc	0.0003254	Paxs	485.47	Joback Method
dvisc	0.0002158	Paxs	534.62	Joback Method
dvisc	0.0001534	Paxs	583.76	Joback Method
dvisc	0.0001150	Paxs	632.90	Joback Method
dvisc	0.0000898	Paxs	682.05	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R233013&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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