6-Methoxythymyl isobutyrate

Inchi: InChI=1S/C15H22O3/c1-9(2)12-8-13(17-6)11(5)7-14(12)18-15(16)10(3)4/h7-10H,1-6H3
InchiKey: JGJKXXDVWAGEOY-UHFFFAOYSA-N
Formula: C15H22O3
SMILES: COc1cc(C(C)C)c(OC(=O)C(C)C)cc1C
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
rinpol	1673.20		NIST Webbook
rinpol	1673.20		NIST Webbook
tb	682.05	K	Joback Method
tc	887.57	K	Joback Method
tf	387.18	K	Joback Method
vc	0.797	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.04	J/mol×K	682.05	Joback Method
cpg	590.62	J/mol×K	716.30	Joback Method
cpg	606.29	J/mol×K	750.56	Joback Method
cpg	621.03	J/mol×K	784.81	Joback Method
cpg	634.86	J/mol×K	819.06	Joback Method
cpg	647.77	J/mol×K	853.31	Joback Method
cpg	659.76	J/mol×K	887.57	Joback Method
dvisc	0.0010114	Pa×s	387.18	Joback Method

dvisc	0.0005382	Pa×s	436.32	Joback Method
dvisc	0.0003254	Pa×s	485.47	Joback Method
dvisc	0.0002158	Pa×s	534.62	Joback Method
dvisc	0.0001534	Pa×s	583.76	Joback Method
dvisc	0.0001150	Pa×s	632.90	Joback Method
dvisc	0.0000898	Pa×s	682.05	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=U413803&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume