3-Methoxy-cuminyl isobutyrate

Inchi: InChI=1S/C15H22O3/c1-10(2)13-7-6-12(8-14(13)17-5)9-18-15(16)11(3)4/h6-8,10-11H,9H
InchiKey: JVOZDVTWETUPPI-UHFFFAOYSA-N
Formula: C15H22O3
SMILES: COc1cc(COC(=O)C(C)C)ccc1C(C)C
Mol. weight [g/mol]: 250.33

Physical Properties

Property code	Value	Unit	Source
gf	-175.23	kJ/mol	Joback Method
hf	-526.92	kJ/mol	Joback Method
hfus	24.80	kJ/mol	Joback Method
hvap	63.37	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.518		Crippen Method
mcvol	211.760	ml/mol	McGowan Method
pc	1870.79	kPa	Joback Method
rinpol	1689.00		NIST Webbook
ripol	2257.00		NIST Webbook
tb	677.07	K	Joback Method
tc	881.74	K	Joback Method
tf	374.66	K	Joback Method
vc	0.797	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.52	J/mol×K	677.07	Joback Method
cpg	591.25	J/mol×K	711.18	Joback Method
cpg	607.04	J/mol×K	745.29	Joback Method
cpg	621.89	J/mol×K	779.41	Joback Method
cpg	635.81	J/mol×K	813.52	Joback Method
cpg	648.81	J/mol×K	847.63	Joback Method
cpg	660.88	J/mol×K	881.74	Joback Method
dvisc	0.0012729	Pa×s	374.66	Joback Method

dvisc	0.0006305	Pa×s	425.06	Joback Method
dvisc	0.0003625	Pa×s	475.46	Joback Method
dvisc	0.0002317	Pa×s	525.87	Joback Method
dvisc	0.0001602	Pa×s	576.27	Joback Method
dvisc	0.0001175	Pa×s	626.67	Joback Method
dvisc	0.0000903	Pa×s	677.07	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=R518304&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