3-Methoxy cuminyl alcohol, isovaleryl ester

Inchi: InChI=1S/C16H24O3/c1-11(2)8-16(17)19-10-13-6-7-14(12(3)4)15(9-13)18-5/h6-7,9,11-1
InchiKey: STRDLKHJGYWBET-UHFFFAOYSA-N
Formula: C16H24O3
SMILES: COc1cc(COC(=O)CC(C)C)ccc1C(C)C
Mol. weight [g/mol]: 264.36

Physical Properties

Property code	Value	Unit	Source
gf	-166.81	kJ/mol	Joback Method
hf	-547.56	kJ/mol	Joback Method
hfus	27.39	kJ/mol	Joback Method
hvap	65.60	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	3.908		Crippen Method
mcvol	225.850	ml/mol	McGowan Method
pc	1724.59	kPa	Joback Method
rinpol	1759.00		NIST Webbook
rinpol	1759.00		NIST Webbook
tb	699.95	K	Joback Method
tc	902.14	K	Joback Method
tf	385.93	K	Joback Method
vc	0.854	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	628.86	J/mol×K	699.95	Joback Method
cpg	645.96	J/mol×K	733.65	Joback Method
cpg	662.08	J/mol×K	767.35	Joback Method
cpg	677.23	J/mol×K	801.04	Joback Method
cpg	691.41	J/mol×K	834.74	Joback Method
cpg	704.64	J/mol×K	868.44	Joback Method
cpg	716.92	J/mol×K	902.14	Joback Method
dvisc	0.0011827	Pa×s	385.93	Joback Method

dvisc	0.0005780	Pa×s	438.27	Joback Method
dvisc	0.0003291	Pa×s	490.60	Joback Method
dvisc	0.0002089	Pa×s	542.94	Joback Method
dvisc	0.0001436	Pa×s	595.28	Joback Method
dvisc	0.0001049	Pa×s	647.61	Joback Method
dvisc	0.0000803	Pa×s	699.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R630870&Units=SI
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

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