

6-Methoxythymyl 2-methylbutyrate

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C16H24O3/c1-7-11(4)16(17)19-15-8-12(5)14(18-6)9-13(15)10(2)3/h8-11H,7H2

RJUMKACVUPSSJD-UHFFFAOYSA-N

C16H24O3

CCC(C)C(=O)Oc1cc(C)c(OC)cc1C(C)C

264.36

Physical Properties

Property code	Value	Unit	Source
gf	-176.44	kJ/mol	Joback Method
hf	-559.03	kJ/mol	Joback Method
hfus	27.00	kJ/mol	Joback Method
hvap	66.26	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	4.079		Crippen Method
mcvol	225.850	ml/mol	McGowan Method
pc	1703.31	kPa	Joback Method
rinpol	1764.50		NIST Webbook
rinpol	1764.50		NIST Webbook
tb	704.93	K	Joback Method
tc	907.94	K	Joback Method
tf	398.45	K	Joback Method
vc	0.854	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	628.41	J/mol×K	704.93	Joback Method
cpg	645.38	J/mol×K	738.77	Joback Method
cpg	661.39	J/mol×K	772.60	Joback Method
cpg	676.44	J/mol×K	806.44	Joback Method
cpg	690.53	J/mol×K	840.27	Joback Method
cpg	703.67	J/mol×K	874.11	Joback Method
cpg	715.86	J/mol×K	907.94	Joback Method
dvisc	0.0009462	Pa×s	398.45	Joback Method

dvisc	0.0004963	Pa×s	449.53	Joback Method
dvisc	0.0002970	Pa×s	500.61	Joback Method
dvisc	0.0001954	Pa×s	551.69	Joback Method
dvisc	0.0001380	Pa×s	602.77	Joback Method
dvisc	0.0001030	Pa×s	653.85	Joback Method
dvisc	0.0000801	Pa×s	704.93	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=U413804&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

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