Pimelic acid, 5-methoxy-3-methylpent-2-yl isobutyl ester

Inchi: InChI=1S/C18H34O5/c1-14(2)13-22-17(19)9-7-6-8-10-18(20)23-16(4)15(3)11-12-21-5/h1

InchiKey: TWAZJLJGYDNEPC-UHFFFAOYSA-N

Formula: C18H34O5

SMILES: COCCC(C)C(C)OC(=O)CCCCCC(=O)OCC(C)C

Mol. weight [g/mol]: 330.46

Physical Properties

Property code	Value	Unit	Source
gf	-479.48	kJ/mol	Joback Method
hf	-1052.51	kJ/mol	Joback Method
hfus	38.57	kJ/mol	Joback Method
hvap	75.22	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	3.740		Crippen Method
mcvol	285.230	ml/mol	McGowan Method
pc	1233.74	kPa	Joback Method
rinpol	2123.00		NIST Webbook
rinpol	2123.00		NIST Webbook
tb	784.92	K	Joback Method
tc	969.58	K	Joback Method
tf	414.17	K	Joback Method
vc	1.091	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	881.95	J/mol×K	784.92	Joback Method
cpg	959.45	J/mol×K	938.80	Joback Method
cpg	946.01	J/mol×K	908.03	Joback Method
cpg	931.55	J/mol×K	877.25	Joback Method
cpg	916.05	J/mol×K	846.47	Joback Method
cpg	899.52	J/mol×K	815.70	Joback Method
cpg	971.86	J/mol×K	969.58	Joback Method
dvisc	0.0000414	Pa×s	784.92	Joback Method

dvisc	0.0000573	Pa×s	723.13	Joback Method
dvisc	0.0000841	Pa×s	661.34	Joback Method
dvisc	0.0001338	Pa×s	599.55	Joback Method
dvisc	0.0002367	Pa×s	537.75	Joback Method
dvisc	0.0004857	Pa×s	475.96	Joback Method
dvisc	0.0012351	Pa×s	414.17	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=U406716&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume