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

Inchi: InChI=1S/C17H32O5/c1-5-12-21-16(18)9-7-6-8-10-17(19)22-15(3)14(2)11-13-20-4/h14-1

InchiKey: LLPZUBAJTFBHJU-UHFFFAOYSA-N

Formula: C17H32O5

SMILES: CCCOC(=O)CCCCCC(=O)OC(C)C(C)CCOC

Mol. weight [g/mol]: 316.43

Physical Properties

Property code	Value	Unit	Source
gf	-485.46	kJ/mol	Joback Method
hf	-1026.59	kJ/mol	Joback Method
hfus	39.50	kJ/mol	Joback Method
hvap	73.38	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	3.494		Crippen Method
mcvol	271.140	ml/mol	McGowan Method
pc	1313.70	kPa	Joback Method
rinpol	2070.00		NIST Webbook
rinpol	2070.00		NIST Webbook
tb	762.48	K	Joback Method
tc	944.32	K	Joback Method
tf	417.90	K	Joback Method
vc	1.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	822.56	J/mol×K	762.48	Joback Method
cpg	839.65	J/mol×K	792.79	Joback Method
cpg	855.78	J/mol×K	823.09	Joback Method
cpg	870.96	J/mol×K	853.40	Joback Method
cpg	885.19	J/mol×K	883.71	Joback Method
cpg	898.47	J/mol×K	914.02	Joback Method
cpg	910.80	J/mol×K	944.32	Joback Method
dvisc	0.0011284	Pa×s	417.90	Joback Method

dvisc	0.0004957	Pa×s	475.33	Joback Method
dvisc	0.0002600	Pa×s	532.76	Joback Method
dvisc	0.0001546	Pa×s	590.19	Joback Method
dvisc	0.0001008	Pa×s	647.62	Joback Method
dvisc	0.0000705	Pa×s	705.05	Joback Method
dvisc	0.0000520	Pa×s	762.48	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=U406715&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