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

Inchi: InChI=1S/C19H36O5/c1-5-6-10-14-23-18(20)11-8-7-9-12-19(21)24-17(3)16(2)13-15-22-4

InchiKey: MVHMWLAPHOTQIW-UHFFFAOYSA-N

Formula: C19H36O5

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

Mol. weight [g/mol]: 344.49

Physical Properties

Property code	Value	Unit	Source
gf	-468.62	kJ/mol	Joback Method
hf	-1067.87	kJ/mol	Joback Method
hfus	44.68	kJ/mol	Joback Method
hvap	77.83	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	4.275		Crippen Method
mcvol	299.320	ml/mol	McGowan Method
pc	1148.32	kPa	Joback Method
rinpol	2260.00		NIST Webbook
rinpol	2260.00		NIST Webbook
tb	808.24	K	Joback Method
tc	993.75	K	Joback Method
tf	440.44	K	Joback Method
vc	1.153	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	941.23	J/mol×K	808.24	Joback Method
cpg	959.02	J/mol×K	839.16	Joback Method
cpg	975.71	J/mol×K	870.08	Joback Method
cpg	991.34	J/mol×K	900.99	Joback Method
cpg	1005.88	J/mol×K	931.91	Joback Method
cpg	1019.37	J/mol×K	962.83	Joback Method
cpg	1031.79	J/mol×K	993.75	Joback Method
dvisc	0.0008930	Pa×s	440.44	Joback Method

dvisc	0.0003849	Pa×s	501.74	Joback Method
dvisc	0.0001993	Pa×s	563.04	Joback Method
dvisc	0.0001174	Pa×s	624.34	Joback Method
dvisc	0.0000760	Pa×s	685.64	Joback Method
dvisc	0.0000529	Pa×s	746.94	Joback Method
dvisc	0.0000389	Pa×s	808.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406719&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

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