Pimelic acid, 5-methoxy-3-methylpent-2-yl 4-methyl-2-pentyl ester

Inchi: InChI=1S/C20H38O5/c1-15(2)14-17(4)24-19(21)10-8-7-9-11-20(22)25-18(5)16(3)12-13-2
InchiKey: HMGRUGQLTQFHOZ-UHFFFAOYSA-N
Formula: C20H38O5
SMILES: COCCC(C)C(C)OC(=O)CCCCCC(=O)OC(C)CC(C)C
Mol. weight [g/mol]: 358.51

Physical Properties

Property code	Value	Unit	Source
gf	-465.08	kJ/mol	Joback Method
hf	-1099.07	kJ/mol	Joback Method
hfus	40.23	kJ/mol	Joback Method
hvap	79.28	kJ/mol	Joback Method
log10ws	-4.75		Crippen Method
logp	4.519		Crippen Method
mcvol	313.410	ml/mol	McGowan Method
pc	1088.50	kPa	Joback Method
rinpol	2221.00		NIST Webbook
tb	830.24	K	Joback Method
tc	1020.18	K	Joback Method
tf	421.71	K	Joback Method
vc	1.198	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1002.76	J/mol×K	830.24	Joback Method
cpg	1021.03	J/mol×K	861.90	Joback Method
cpg	1038.10	J/mol×K	893.55	Joback Method
cpg	1053.99	J/mol×K	925.21	Joback Method
cpg	1068.69	J/mol×K	956.87	Joback Method
cpg	1082.22	J/mol×K	988.53	Joback Method
cpg	1094.59	J/mol×K	1020.18	Joback Method
dvisc	0.0011834	Pa×s	421.71	Joback Method
dvisc	0.0004116	Pa×s	489.80	Joback Method

dvisc	0.0001853	Pa×s	557.89	Joback Method
dvisc	0.0000992	Pa×s	625.98	Joback Method
dvisc	0.0000600	Pa×s	694.06	Joback Method
dvisc	0.0000398	Pa×s	762.15	Joback Method
dvisc	0.0000282	Pa×s	830.24	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=U406718&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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