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

Inchi: InChI=1S/C25H48O5/c1-5-6-7-8-9-10-11-12-16-20-29-24(26)17-14-13-15-18-25(27)30-2
InchiKey: VHXKKIGQFQANQS-UHFFFAOYSA-N
Formula: C25H48O5
SMILES: CCCCCCCCCCCOC(=O)CCCCCC(=O)OC(C)C(C)CCOC
Mol. weight [g/mol]: 428.65

Physical Properties

Property code	Value	Unit	Source
gf	-418.10	kJ/mol	Joback Method
hf	-1191.71	kJ/mol	Joback Method
hfus	60.22	kJ/mol	Joback Method
hvap	91.19	kJ/mol	Joback Method
log10ws	-6.97		Crippen Method
logp	6.615		Crippen Method
mcvol	383.860	ml/mol	McGowan Method
pc	803.88	kPa	Joback Method
rinpol	2847.00		NIST Webbook
rinpol	2847.00		NIST Webbook
tb	945.52	K	Joback Method
tc	1161.79	K	Joback Method
tf	508.06	K	Joback Method
vc	1.490	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1313.99	J/mol×K	945.52	Joback Method
cpg	1397.45	J/mol×K	1125.75	Joback Method
cpg	1384.12	J/mol×K	1089.70	Joback Method
cpg	1369.14	J/mol×K	1053.66	Joback Method
cpg	1352.48	J/mol×K	1017.61	Joback Method
cpg	1334.10	J/mol×K	981.57	Joback Method
cpg	1409.15	J/mol×K	1161.79	Joback Method
dvisc	0.0000154	Pa×s	945.52	Joback Method

dvisc	0.0000212	Pa×s	872.61	Joback Method
dvisc	0.0000309	Pa×s	799.70	Joback Method
dvisc	0.0000486	Pa×s	726.79	Joback Method
dvisc	0.0000843	Pa×s	653.88	Joback Method
dvisc	0.0001683	Pa×s	580.97	Joback Method
dvisc	0.0004093	Pa×s	508.06	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406724&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