Pimelic acid, 3-methyl-2-pentyl undecyl ester

Inchi: InChI=1S/C24H46O4/c1-5-7-8-9-10-11-12-13-17-20-27-23(25)18-15-14-16-19-24(26)28-
InchiKey: QVSHCHISSSWSBW-UHFFFAOYSA-N
Formula: C24H46O4
SMILES: CCCCCCCCCCCOC(=O)CCCCCC(=O)OC(C)C(C)CC
Mol. weight [g/mol]: 398.62

Physical Properties

Property code	Value	Unit	Source
gf	-321.52	kJ/mol	Joback Method
hf	-1038.85	kJ/mol	Joback Method
hfus	56.44	kJ/mol	Joback Method
hvap	86.55	kJ/mol	Joback Method
log10ws	-7.46		Crippen Method
logp	6.989		Crippen Method
mcvol	363.900	ml/mol	McGowan Method
pc	857.97	kPa	Joback Method
rinpol	2654.00		NIST Webbook
rinpol	2654.00		NIST Webbook
tb	900.22	K	Joback Method
tc	1102.59	K	Joback Method
tf	474.56	K	Joback Method
vc	1.415	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1218.42	J/mol×K	900.22	Joback Method
cpg	1304.81	J/mol×K	1068.86	Joback Method
cpg	1290.22	J/mol×K	1035.14	Joback Method
cpg	1274.32	J/mol×K	1001.41	Joback Method
cpg	1257.07	J/mol×K	967.68	Joback Method
cpg	1238.45	J/mol×K	933.95	Joback Method
cpg	1318.12	J/mol×K	1102.59	Joback Method
dvisc	0.0000246	Pa×s	900.22	Joback Method

dvisc	0.0000339	Pa×s	829.28	Joback Method
dvisc	0.0000496	Pa×s	758.33	Joback Method
dvisc	0.0000786	Pa×s	687.39	Joback Method
dvisc	0.0001385	Pa×s	616.45	Joback Method
dvisc	0.0002826	Pa×s	545.50	Joback Method
dvisc	0.0007142	Pa×s	474.56	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=U406601&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

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