

Pimelic acid, 2-(2-methoxyethyl)hexyl undecyl ester

Inchi:	InChI=1S/C27H52O5/c1-4-6-8-9-10-11-12-13-17-22-31-26(28)19-15-14-16-20-27(29)32-
InchiKey:	CLOWARDPCMVUTG-UHFFFAOYSA-N
Formula:	C27H52O5
SMILES:	CCCCCCCCCOC(=O)CCCCCC(=O)OCC(CCCC)CCOC
Mol. weight [g/mol]:	456.70

Physical Properties

Property code	Value	Unit	Source
gf	-398.82	kJ/mol	Joback Method
hf	-1227.71	kJ/mol	Joback Method
hfus	68.92	kJ/mol	Joback Method
hvap	96.03	kJ/mol	Joback Method
log10ws	-7.70		Crippen Method
logp	7.397		Crippen Method
mcvol	412.040	ml/mol	McGowan Method
pc	719.91	kPa	Joback Method
rinpol	3046.00		NIST Webbook
rinpol	3046.00		NIST Webbook
tb	991.72	K	Joback Method
tc	1229.04	K	Joback Method
tf	545.60	K	Joback Method
vc	1.607	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1441.72	J/molxK	991.72	Joback Method
cpg	1463.04	J/molxK	1031.27	Joback Method
cpg	1482.22	J/molxK	1070.83	Joback Method
cpg	1499.30	J/molxK	1110.38	Joback Method
cpg	1514.33	J/molxK	1149.93	Joback Method
cpg	1527.37	J/molxK	1189.49	Joback Method
cpg	1538.45	J/molxK	1229.04	Joback Method
dvisc	0.0002711	Paxs	545.60	Joback Method

dvisc	0.0001189	Paxs	619.95	Joback Method
dvisc	0.0000622	Paxs	694.31	Joback Method
dvisc	0.0000369	Paxs	768.66	Joback Method
dvisc	0.0000240	Paxs	843.01	Joback Method
dvisc	0.0000167	Paxs	917.37	Joback Method
dvisc	0.0000123	Paxs	991.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406750&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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

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