

Pimelic acid, phenethyl undecyl ester

Inchi:	InChI=1S/C26H42O4/c1-2-3-4-5-6-7-8-9-16-22-29-25(27)19-14-11-15-20-26(28)30-23-2
InchiKey:	LIJBHUXCFIKBEC-UHFFFAOYSA-N
Formula:	C26H42O4
SMILES:	CCCCCCCCCOC(=O)CCCCC(=O)OCCc1ccccc1
Mol. weight [g/mol]:	418.61

Physical Properties

Property code	Value	Unit	Source
gf	-187.39	kJ/mol	Joback Method
hf	-833.04	kJ/mol	Joback Method
hfus	62.71	kJ/mol	Joback Method
hvap	94.06	kJ/mol	Joback Method
log10ws	-7.53		Crippen Method
logp	6.797		Crippen Method
mcvol	368.320	ml/mol	McGowan Method
pc	923.30	kPa	Joback Method
rinpol	3173.00		NIST Webbook
rinpol	3173.00		NIST Webbook
tb	973.54	K	Joback Method
tc	1192.35	K	Joback Method
tf	553.52	K	Joback Method
vc	1.431	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1244.21	J/molxK	973.54	Joback Method
cpg	1318.16	J/molxK	1155.88	Joback Method
cpg	1306.17	J/molxK	1119.41	Joback Method
cpg	1292.83	J/molxK	1082.94	Joback Method
cpg	1278.10	J/molxK	1046.48	Joback Method
cpg	1261.91	J/molxK	1010.01	Joback Method
cpg	1328.87	J/molxK	1192.35	Joback Method
dvisc	0.0000223	Paxs	973.54	Joback Method

dvisc	0.0000295	Paxs	903.54	Joback Method
dvisc	0.0000409	Paxs	833.53	Joback Method
dvisc	0.0000603	Paxs	763.53	Joback Method
dvisc	0.0000962	Paxs	693.53	Joback Method
dvisc	0.0001703	Paxs	623.52	Joback Method
dvisc	0.0003484	Paxs	553.52	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U416503&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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