Pimelic acid, 3-phenylpropyl undecyl ester

Inchi: InChI=1S/C27H44O4/c1-2-3-4-5-6-7-8-9-16-23-30-26(28)21-14-11-15-22-27(29)31-24-17
InchiKey: HEBGLWLPKCTUFO-UHFFFAOYSA-N
Formula: C27H44O4
SMILES: CCCCCCCCCCCOC(=O)CCCCCC(=O)OCCCc1ccccc1
Mol. weight [g/mol]: 432.64

Physical Properties

Property code	Value	Unit	Source
gf	-178.97	kJ/mol	Joback Method
hf	-853.68	kJ/mol	Joback Method
hfus	65.30	kJ/mol	Joback Method
hvap	96.28	kJ/mol	Joback Method
log10ws	-7.95		Crippen Method
logp	7.187		Crippen Method
mcvol	382.410	ml/mol	McGowan Method
pc	871.71	kPa	Joback Method
rinpol	3285.00		NIST Webbook
rinpol	3285.00		NIST Webbook
tb	996.42	K	Joback Method
tc	1221.91	K	Joback Method
tf	564.79	K	Joback Method
vc	1.488	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1307.01	J/mol×K	996.42	Joback Method
cpg	1325.04	J/mol×K	1034.00	Joback Method
cpg	1341.46	J/mol×K	1071.58	Joback Method
cpg	1356.33	J/mol×K	1109.17	Joback Method
cpg	1369.72	J/mol×K	1146.75	Joback Method
cpg	1381.69	J/mol×K	1184.33	Joback Method
cpg	1392.31	J/mol×K	1221.91	Joback Method
dvisc	0.0003070	Pa×s	564.79	Joback Method

dvisc	0.0001487	Pa×s	636.73	Joback Method
dvisc	0.0000835	Pa×s	708.67	Joback Method
dvisc	0.0000521	Pa×s	780.61	Joback Method
dvisc	0.0000352	Pa×s	852.54	Joback Method
dvisc	0.0000253	Pa×s	924.48	Joback Method
dvisc	0.0000191	Pa×s	996.42	Joback Method

Sources

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=U416518&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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