Pimelic acid, 2-methylphenyl tridecyl ester

Inchi: InChI=1S/C27H44O4/c1-3-4-5-6-7-8-9-10-11-12-18-23-30-26(28)21-14-13-15-22-27(29)3
InchiKey: TZVNDNRPERUGJT-UHFFFAOYSA-N
Formula: C27H44O4
SMILES: CCCCCCCCCCCCCOC(=O)CCCCCC(=O)Oc1ccccc1C
Mol. weight [g/mol]: 432.64

Physical Properties

Property code	Value	Unit	Source
gf	-188.60	kJ/mol	Joback Method
hf	-865.15	kJ/mol	Joback Method
hfus	64.91	kJ/mol	Joback Method
hvap	96.95	kJ/mol	Joback Method
log10ws	-8.66		Crippen Method
logp	7.705		Crippen Method
mcvol	382.410	ml/mol	McGowan Method
pc	864.04	kPa	Joback Method
rinpol	2668.00		NIST Webbook
rinpol	2668.00		NIST Webbook
tb	1001.40	K	Joback Method
tc	1228.17	K	Joback Method
tf	577.31	K	Joback Method
vc	1.488	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1306.45	J/mol×K	1001.40	Joback Method
cpg	1324.35	J/mol×K	1039.19	Joback Method
cpg	1340.59	J/mol×K	1076.99	Joback Method
cpg	1355.23	J/mol×K	1114.78	Joback Method
cpg	1368.34	J/mol×K	1152.58	Joback Method
cpg	1379.97	J/mol×K	1190.37	Joback Method
cpg	1390.19	J/mol×K	1228.17	Joback Method
dvisc	0.0002685	Pa×s	577.31	Joback Method

dvisc	0.0001367	Pa×s	647.99	Joback Method
dvisc	0.0000795	Pa×s	718.67	Joback Method
dvisc	0.0000510	Pa×s	789.36	Joback Method
dvisc	0.0000351	Pa×s	860.04	Joback Method
dvisc	0.0000256	Pa×s	930.72	Joback Method
dvisc	0.0000195	Pa×s	1001.40	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=U416493&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