Pimelic acid, 2-methoxyphenyl tridecyl ester

Inchi: InChI=1S/C27H44O5/c1-3-4-5-6-7-8-9-10-11-12-18-23-31-26(28)21-14-13-15-22-27(29)3
InchiKey: HQVCVMXWQWFLST-UHFFFAOYSA-N
Formula: C27H44O5
SMILES: CCCCCCCCCCCCCOC(=O)CCCCCC(=O)Oc1ccccc1OC
Mol. weight [g/mol]: 448.64

Physical Properties

Property code	Value	Unit	Source
gf	-293.60	kJ/mol	Joback Method
hf	-997.37	kJ/mol	Joback Method
hfus	66.10	kJ/mol	Joback Method
hvap	99.36	kJ/mol	Joback Method
log10ws	-8.30		Crippen Method
logp	7.405		Crippen Method
mcvol	388.280	ml/mol	McGowan Method
pc	855.46	kPa	Joback Method
rinpol	2899.00		NIST Webbook
tb	1023.82	K	Joback Method
tc	1258.07	K	Joback Method
tf	599.54	K	Joback Method
vc	1.506	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1335.61	J/mol×K	1023.82	Joback Method
cpg	1352.63	J/mol×K	1062.86	Joback Method
cpg	1367.73	J/mol×K	1101.90	Joback Method
cpg	1380.96	J/mol×K	1140.94	Joback Method
cpg	1392.36	J/mol×K	1179.99	Joback Method
cpg	1401.98	J/mol×K	1219.03	Joback Method
cpg	1409.86	J/mol×K	1258.07	Joback Method
dvisc	0.0001845	Pa×s	599.54	Joback Method
dvisc	0.0000963	Pa×s	670.25	Joback Method

dvisc	0.0000569	Pa×s	740.97	Joback Method
dvisc	0.0000369	Pa×s	811.68	Joback Method
dvisc	0.0000256	Pa×s	882.39	Joback Method
dvisc	0.0000188	Pa×s	953.11	Joback Method
dvisc	0.0000144	Pa×s	1023.82	Joback Method

Sources

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=U416533&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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