Pimelic acid, 2-methoxyphenyl octyl ester

Inchi: InChI=1S/C22H34O5/c1-3-4-5-6-7-13-18-26-21(23)16-9-8-10-17-22(24)27-20-15-12-11-1
InchiKey: MPMVIGAVTKDOIQ-UHFFFAOYSA-N
Formula: C22H34O5
SMILES: CCCCCCCCOC(=O)CCCCCC(=O)Oc1ccccc1OC
Mol. weight [g/mol]: 378.50

Physical Properties

Property code	Value	Unit	Source
gf	-335.70	kJ/mol	Joback Method
hf	-894.17	kJ/mol	Joback Method
hfus	53.15	kJ/mol	Joback Method
hvap	88.23	kJ/mol	Joback Method
log10ws	-6.21		Crippen Method
logp	5.455		Crippen Method
mcvol	317.830	ml/mol	McGowan Method
pc	1157.71	kPa	Joback Method
rinpol	2859.00		NIST Webbook
rinpol	2859.00		NIST Webbook
tb	909.42	K	Joback Method
tc	1115.54	K	Joback Method
tf	543.19	K	Joback Method
vc	1.226	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1027.01	J/mol×K	909.42	Joback Method
cpg	1093.70	J/mol×K	1081.18	Joback Method
cpg	1082.99	J/mol×K	1046.83	Joback Method
cpg	1070.99	J/mol×K	1012.48	Joback Method
cpg	1057.67	J/mol×K	978.13	Joback Method
cpg	1043.01	J/mol×K	943.77	Joback Method
cpg	1103.12	J/mol×K	1115.54	Joback Method
dvisc	0.0000307	Pa×s	909.42	Joback Method

dvisc	0.0000397	Pa×s	848.38	Joback Method
dvisc	0.0000532	Pa×s	787.34	Joback Method
dvisc	0.0000751	Pa×s	726.31	Joback Method
dvisc	0.0001129	Pa×s	665.27	Joback Method
dvisc	0.0001841	Pa×s	604.23	Joback Method
dvisc	0.0003352	Pa×s	543.19	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=U416528&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