Pimelic acid, 2-methoxyphenyl undecyl ester

Inchi: InChI=1S/C25H40O5/c1-3-4-5-6-7-8-9-10-16-21-29-24(26)19-12-11-13-20-25(27)30-23-1
InchiKey: GHBSEHUCLQZXTO-UHFFFAOYSA-N
Formula: C25H40O5
SMILES: CCCCCCCCCCCOC(=O)CCCCCC(=O)Oc1ccccc1OC
Mol. weight [g/mol]: 420.58

Physical Properties

Property code	Value	Unit	Source
gf	-310.44	kJ/mol	Joback Method
hf	-956.09	kJ/mol	Joback Method
hfus	60.92	kJ/mol	Joback Method
hvap	94.90	kJ/mol	Joback Method
log10ws	-7.47		Crippen Method
logp	6.625		Crippen Method
mcvol	360.100	ml/mol	McGowan Method
pc	960.29	kPa	Joback Method
rinpol	3163.00		NIST Webbook
rinpol	3163.00		NIST Webbook
tb	978.06	K	Joback Method
tc	1197.84	K	Joback Method
tf	577.00	K	Joback Method
vc	1.393	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1210.94	J/mol×K	978.06	Joback Method
cpg	1227.53	J/mol×K	1014.69	Joback Method
cpg	1242.47	J/mol×K	1051.32	Joback Method
cpg	1255.79	J/mol×K	1087.95	Joback Method
cpg	1267.54	J/mol×K	1124.58	Joback Method
cpg	1277.74	J/mol×K	1161.21	Joback Method
cpg	1286.41	J/mol×K	1197.84	Joback Method
dvisc	0.0002363	Pa×s	577.00	Joback Method

dvisc	0.0001258	Pa×s	643.84	Joback Method
dvisc	0.0000754	Pa×s	710.69	Joback Method
dvisc	0.0000493	Pa×s	777.53	Joback Method
dvisc	0.0000345	Pa×s	844.37	Joback Method
dvisc	0.0000255	Pa×s	911.22	Joback Method
dvisc	0.0000196	Pa×s	978.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416531&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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