Pimelic acid, 2-methoxyphenyl pentyl ester

Inchi: InChI=1S/C19H28O5/c1-3-4-10-15-23-18(20)13-6-5-7-14-19(21)24-17-12-9-8-11-16(17)2
InchiKey: XPFFDDRXYLQGQS-UHFFFAOYSA-N
Formula: C19H28O5
SMILES: CCCCCOC(=O)CCCCCC(=O)Oc1ccccc1OC
Mol. weight [g/mol]: 336.42

Physical Properties

Property code	Value	Unit	Source
gf	-360.96	kJ/mol	Joback Method
hf	-832.25	kJ/mol	Joback Method
hfus	45.38	kJ/mol	Joback Method
hvap	81.55	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	4.284		Crippen Method
mcvol	275.560	ml/mol	McGowan Method
pc	1422.92	kPa	Joback Method
rinpol	2558.00		NIST Webbook
tb	840.78	K	Joback Method
tc	1041.20	K	Joback Method
tf	509.38	K	Joback Method
vc	1.058	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	848.17	J/mol×K	840.78	Joback Method
cpg	863.62	J/mol×K	874.18	Joback Method
cpg	877.92	J/mol×K	907.59	Joback Method
cpg	891.07	J/mol×K	940.99	Joback Method
cpg	903.09	J/mol×K	974.39	Joback Method
cpg	913.97	J/mol×K	1007.79	Joback Method
cpg	923.73	J/mol×K	1041.20	Joback Method
dvisc	0.0004609	Pa×s	509.38	Joback Method
dvisc	0.0002620	Pa×s	564.61	Joback Method

dvisc	0.0001648	Pa×s	619.85	Joback Method
dvisc	0.0001118	Pa×s	675.08	Joback Method
dvisc	0.0000804	Pa×s	730.31	Joback Method
dvisc	0.0000606	Pa×s	785.55	Joback Method
dvisc	0.0000474	Pa×s	840.78	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416525&Units=SI

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