Pimelic acid, di(2-methoxyphenyl) ester

Inchi: InChI=1S/C21H24O6/c1-24-16-10-6-8-12-18(16)26-20(22)14-4-3-5-15-21(23)27-19-13-9
InchiKey: LPDUDADAIIEINQ-UHFFFAOYSA-N
Formula: C21H24O6
SMILES: COc1ccccc1OC(=O)CCCCCC(=O)Oc1ccccc1OC
Mol. weight [g/mol]: 372.41

Physical Properties

Property code	Value	Unit	Source
gf	-346.34	kJ/mol	Joback Method
hf	-780.69	kJ/mol	Joback Method
hfus	45.40	kJ/mol	Joback Method
hvap	91.35	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.165		Crippen Method
mcvol	285.850	ml/mol	McGowan Method
pc	1545.13	kPa	Joback Method
rinpol	2317.00		NIST Webbook
rinpol	2317.00		NIST Webbook
tb	940.62	K	Joback Method
tc	1164.12	K	Joback Method
tf	593.09	K	Joback Method
vc	1.079	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	892.45	J/mol×K	940.62	Joback Method
cpg	904.95	J/mol×K	977.87	Joback Method
cpg	915.90	J/mol×K	1015.12	Joback Method
cpg	925.31	J/mol×K	1052.37	Joback Method
cpg	933.16	J/mol×K	1089.62	Joback Method
cpg	939.47	J/mol×K	1126.87	Joback Method
cpg	944.24	J/mol×K	1164.12	Joback Method
dvisc	0.0002084	Pa×s	593.09	Joback Method

dvisc	0.0001283	Pa×s	651.01	Joback Method
dvisc	0.0000855	Pa×s	708.93	Joback Method
dvisc	0.0000606	Pa×s	766.86	Joback Method
dvisc	0.0000451	Pa×s	824.78	Joback Method
dvisc	0.0000348	Pa×s	882.70	Joback Method
dvisc	0.0000278	Pa×s	940.62	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=U416534&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