Pimelic acid, di(3-phenylpropyl) ester

Inchi: InChI=1S/C25H32O4/c26-24(28-20-10-16-22-12-4-1-5-13-22)18-8-3-9-19-25(27)29-21-1
InchiKey: LRPSWUFYPYNCOV-UHFFFAOYSA-N
Formula: C25H32O4
SMILES: O=C(CCCCCC(=O)OCCCc1ccccc1)OCCCc1ccccc1
Mol. weight [g/mol]: 396.52

Physical Properties

Property code	Value	Unit	Source
gf	-83.40	kJ/mol	Joback Method
hf	-575.87	kJ/mol	Joback Method
hfus	54.16	kJ/mol	Joback Method
hvap	94.11	kJ/mol	Joback Method
log10ws	-6.22		Crippen Method
logp	5.289		Crippen Method
mcvol	330.470	ml/mol	McGowan Method
pc	1219.14	kPa	Joback Method
rinpol	2262.00		NIST Webbook
rinpol	2262.00		NIST Webbook
tb	977.34	K	Joback Method
tc	1200.89	K	Joback Method
tf	568.67	K	Joback Method
vc	1.268	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1078.01	J/mol×K	977.34	Joback Method
cpg	1092.66	J/mol×K	1014.60	Joback Method
cpg	1105.92	J/mol×K	1051.86	Joback Method
cpg	1117.86	J/mol×K	1089.11	Joback Method
cpg	1128.53	J/mol×K	1126.37	Joback Method
cpg	1138.01	J/mol×K	1163.63	Joback Method
cpg	1146.35	J/mol×K	1200.89	Joback Method
dvisc	0.0003429	Pa×s	568.67	Joback Method

dvisc	0.0001786	Pa×s	636.78	Joback Method
dvisc	0.0001055	Pa×s	704.89	Joback Method
dvisc	0.0000684	Pa×s	773.00	Joback Method
dvisc	0.0000476	Pa×s	841.12	Joback Method
dvisc	0.0000349	Pa×s	909.23	Joback Method
dvisc	0.0000268	Pa×s	977.34	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=U416520&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