Pimelic acid, (2-(cyclohexenyl-3)-1-phenyl)ethyl isobutyl ester

Inchi: InChI=1S/C25H36O4/c1-20(2)19-28-24(26)16-10-5-11-17-25(27)29-23(22-14-8-4-9-15-2
InchiKey: MZPKZSHKVVDOAE-UHFFFAOYSA-N
Formula: C25H36O4
SMILES: CC(C)COC(=O)CCCCCC(=O)OC(CC1C=CCCC1)c1ccccc1
Mol. weight [g/mol]: 400.55

Physical Properties

Property code	Value	Unit	Source
gf	-146.28	kJ/mol	Joback Method
hf	-710.86	kJ/mol	Joback Method
hfus	46.13	kJ/mol	Joback Method
hvap	91.78	kJ/mol	Joback Method
log10ws	-6.84		Crippen Method
logp	6.167		Crippen Method
mcvol	339.070	ml/mol	McGowan Method
pc	1158.50	kPa	Joback Method
rinpol	2880.00		NIST Webbook
rinpol	2880.00		NIST Webbook
tb	968.49	K	Joback Method
tc	1192.00	K	Joback Method
tf	520.39	K	Joback Method
vc	1.282	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1146.61	J/mol×K	968.49	Joback Method
cpg	1162.86	J/mol×K	1005.74	Joback Method
cpg	1177.48	J/mol×K	1042.99	Joback Method
cpg	1190.53	J/mol×K	1080.25	Joback Method
cpg	1202.06	J/mol×K	1117.50	Joback Method
cpg	1212.15	J/mol×K	1154.75	Joback Method
cpg	1220.84	J/mol×K	1192.00	Joback Method
dvisc	0.0005624	Pa×s	520.39	Joback Method

dvisc	0.0002396	Pa×s	595.07	Joback Method
dvisc	0.0001234	Pa×s	669.76	Joback Method
dvisc	0.0000727	Pa×s	744.44	Joback Method
dvisc	0.0000471	Pa×s	819.12	Joback Method
dvisc	0.0000328	Pa×s	893.81	Joback Method
dvisc	0.0000242	Pa×s	968.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416465&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

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