Pimelic acid, (2-(cyclohexenyl-3)-1-phenyl)ethyl 4-methyl-2-pentyl ester

Inchi: InChI=1S/C27H40O4/c1-21(2)19-22(3)30-26(28)17-11-6-12-18-27(29)31-25(24-15-9-5-1
InchiKey: GYBQNAJPOCOMCO-UHFFFAOYSA-N
Formula: C27H40O4
SMILES: CC(C)CC(C)OC(=O)CCCCCC(=O)OC(CC1C=CCCC1)c1ccccc1
Mol. weight [g/mol]: 428.60

Physical Properties

Property code	Value	Unit	Source
gf	-131.88	kJ/mol	Joback Method
hf	-757.42	kJ/mol	Joback Method
hfus	47.79	kJ/mol	Joback Method
hvap	95.84	kJ/mol	Joback Method
log10ws	-7.79		Crippen Method
logp	6.946		Crippen Method
mcvol	367.250	ml/mol	McGowan Method
pc	1025.97	kPa	Joback Method
rinpol	2979.00		NIST Webbook
rinpol	2979.00		NIST Webbook
tb	1013.81	K	Joback Method
tc	1243.07	K	Joback Method
tf	527.93	K	Joback Method
vc	1.389	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1270.46	J/mol×K	1013.81	Joback Method
cpg	1286.57	J/mol×K	1052.02	Joback Method
cpg	1300.93	J/mol×K	1090.23	Joback Method
cpg	1313.62	J/mol×K	1128.44	Joback Method
cpg	1324.70	J/mol×K	1166.65	Joback Method
cpg	1334.25	J/mol×K	1204.86	Joback Method
cpg	1342.35	J/mol×K	1243.07	Joback Method
dvisc	0.0004923	Pa×s	527.93	Joback Method

dvisc	0.0001907	Pa×s	608.91	Joback Method
dvisc	0.0000923	Pa×s	689.89	Joback Method
dvisc	0.0000520	Pa×s	770.87	Joback Method
dvisc	0.0000327	Pa×s	851.85	Joback Method
dvisc	0.0000223	Pa×s	932.83	Joback Method
dvisc	0.0000161	Pa×s	1013.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416467&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