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

Inchi: InChI=1S/C27H40O4/c1-2-3-4-14-21-30-26(28)19-12-7-13-20-27(29)31-25(24-17-10-6-1

InchiKey: NICGJIKDWRXTGV-UHFFFAOYSA-N

Formula: C27H40O4

SMILES: CCCCCCOC(=O)CCCCCC(=O)OC(CC1C=CCCC1)c1ccccc1

Mol. weight [g/mol]: 428.60

Physical Properties

Property code	Value	Unit	Source
gf	-127.00	kJ/mol	Joback Method
hf	-746.86	kJ/mol	Joback Method
hfus	54.84	kJ/mol	Joback Method
hvap	96.62	kJ/mol	Joback Method
log10ws	-7.92		Crippen Method
logp	7.091		Crippen Method
mcvol	367.250	ml/mol	McGowan Method
pc	1015.53	kPa	Joback Method
rinpol	3173.00		NIST Webbook
rinpol	3173.00		NIST Webbook
tb	1014.69	K	Joback Method
tc	1242.91	K	Joback Method
tf	557.93	K	Joback Method
vc	1.401	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1269.83	J/mol×K	1014.69	Joback Method
cpg	1286.01	J/mol×K	1052.73	Joback Method
cpg	1300.48	J/mol×K	1090.76	Joback Method
cpg	1313.32	J/mol×K	1128.80	Joback Method
cpg	1324.60	J/mol×K	1166.84	Joback Method
cpg	1334.39	J/mol×K	1204.87	Joback Method
cpg	1342.77	J/mol×K	1242.91	Joback Method
dvisc	0.0003830	Pa×s	557.93	Joback Method

dvisc	0.0001732	Pa×s	634.06	Joback Method
dvisc	0.0000928	Pa×s	710.18	Joback Method
dvisc	0.0000561	Pa×s	786.31	Joback Method
dvisc	0.0000371	Pa×s	862.44	Joback Method
dvisc	0.0000262	Pa×s	938.56	Joback Method
dvisc	0.0000195	Pa×s	1014.69	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=U416469&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

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