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

Inchi: InChI=1S/C26H38O4/c1-2-3-13-20-29-25(27)18-11-6-12-19-26(28)30-24(23-16-9-5-10-1

InchiKey: HCVFYGTWDIODHF-UHFFFAOYSA-N

Formula: C26H38O4

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

Mol. weight [g/mol]: 414.58

Physical Properties

Property code	Value	Unit	Source
gf	-135.42	kJ/mol	Joback Method
hf	-726.22	kJ/mol	Joback Method
hfus	52.24	kJ/mol	Joback Method
hvap	94.39	kJ/mol	Joback Method
log10ws	-7.50		Crippen Method
logp	6.701		Crippen Method
mcvol	353.160	ml/mol	McGowan Method
pc	1080.64	kPa	Joback Method
rinpol	3077.00		NIST Webbook
rinpol	3077.00		NIST Webbook
tb	991.81	K	Joback Method
tc	1216.58	K	Joback Method
tf	546.66	K	Joback Method
vc	1.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1207.84	J/mol×K	991.81	Joback Method
cpg	1272.94	J/mol×K	1179.12	Joback Method
cpg	1262.95	J/mol×K	1141.66	Joback Method
cpg	1251.52	J/mol×K	1104.19	Joback Method
cpg	1238.56	J/mol×K	1066.73	Joback Method
cpg	1224.02	J/mol×K	1029.27	Joback Method
cpg	1281.54	J/mol×K	1216.58	Joback Method
dvisc	0.0000228	Pa×s	991.81	Joback Method

dvisc	0.0000306	Pa×s	917.62	Joback Method
dvisc	0.0000431	Pa×s	843.43	Joback Method
dvisc	0.0000650	Pa×s	769.24	Joback Method
dvisc	0.0001071	Pa×s	695.04	Joback Method
dvisc	0.0001988	Pa×s	620.85	Joback Method
dvisc	0.0004361	Pa×s	546.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416468&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