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

Inchi: InChI=1S/C28H42O4/c1-2-3-4-5-15-22-31-27(29)20-13-8-14-21-28(30)32-26(25-18-11-7
InchiKey: ZQRWJDWDKRWOPU-UHFFFAOYSA-N
Formula: C28H42O4
SMILES: CCCCCCCOC(=O)CCCCCC(=O)OC(CC1C=CCCC1)c1ccccc1
Mol. weight [g/mol]: 442.63

Physical Properties

Property code	Value	Unit	Source
gf	-118.58	kJ/mol	Joback Method
hf	-767.50	kJ/mol	Joback Method
hfus	57.42	kJ/mol	Joback Method
hvap	98.84	kJ/mol	Joback Method
log10ws	-8.34		Crippen Method
logp	7.481		Crippen Method
mcvol	381.340	ml/mol	McGowan Method
pc	956.14	kPa	Joback Method
rinpol	2246.00		NIST Webbook
rinpol	2246.00		NIST Webbook
tb	1037.57	K	Joback Method
tc	1270.28	K	Joback Method
tf	569.20	K	Joback Method
vc	1.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1332.16	J/mol×K	1037.57	Joback Method
cpg	1348.36	J/mol×K	1076.36	Joback Method
cpg	1362.78	J/mol×K	1115.14	Joback Method
cpg	1375.51	J/mol×K	1153.93	Joback Method
cpg	1386.62	J/mol×K	1192.71	Joback Method
cpg	1396.21	J/mol×K	1231.50	Joback Method
cpg	1404.35	J/mol×K	1270.28	Joback Method
dvisc	0.0003356	Pa×s	569.20	Joback Method

dvisc	0.0001505	Pa×s	647.26	Joback Method
dvisc	0.0000803	Pa×s	725.32	Joback Method
dvisc	0.0000483	Pa×s	803.39	Joback Method
dvisc	0.0000319	Pa×s	881.45	Joback Method
dvisc	0.0000225	Pa×s	959.51	Joback Method
dvisc	0.0000167	Pa×s	1037.57	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416470&Units=SI

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