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

Inchi: InChI=1S/C23H32O4/c1-2-26-22(24)16-10-5-11-17-23(25)27-21(20-14-8-4-9-15-20)18-1

InchiKey: VLDBULPGJQUXLA-UHFFFAOYSA-N

Formula: C23H32O4

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

Mol. weight [g/mol]: 372.50

Physical Properties

Property code	Value	Unit	Source
gf	-160.68	kJ/mol	Joback Method
hf	-664.30	kJ/mol	Joback Method
hfus	44.47	kJ/mol	Joback Method
hvap	87.71	kJ/mol	Joback Method
log10ws	-6.24		Crippen Method
logp	5.531		Crippen Method
mcvol	310.890	ml/mol	McGowan Method
pc	1318.48	kPa	Joback Method
rinpol	2780.00		NIST Webbook
rinpol	2780.00		NIST Webbook
tb	923.17	K	Joback Method
tc	1143.17	K	Joback Method
tf	512.85	K	Joback Method
vc	1.177	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1024.30	J/mol×K	923.17	Joback Method
cpg	1040.63	J/mol×K	959.84	Joback Method
cpg	1055.42	J/mol×K	996.50	Joback Method
cpg	1068.72	J/mol×K	1033.17	Joback Method
cpg	1080.59	J/mol×K	1069.84	Joback Method
cpg	1091.09	J/mol×K	1106.50	Joback Method
cpg	1100.25	J/mol×K	1143.17	Joback Method
dvisc	0.0006331	Pa×s	512.85	Joback Method

dvisc	0.0002961	Pa×s	581.24	Joback Method
dvisc	0.0001625	Pa×s	649.62	Joback Method
dvisc	0.0001000	Pa×s	718.01	Joback Method
dvisc	0.0000669	Pa×s	786.40	Joback Method
dvisc	0.0000478	Pa×s	854.78	Joback Method
dvisc	0.0000359	Pa×s	923.17	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=U416463&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