

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

Inchi: InChI=1S/C24H34O4/c1-2-18-27-23(25)16-10-5-11-17-24(26)28-22(21-14-8-4-9-15-21)1
InchiKey: FRXMXGBNISBSFE-UHFFFAOYSA-N
Formula: C24H34O4
SMILES: CCCOC(=O)CCCCC(=O)OC(CC1C=CCCC1)c1ccccc1
Mol. weight [g/mol]: 386.52

Physical Properties

Property code	Value	Unit	Source
gf	-152.26	kJ/mol	Joback Method
hf	-684.94	kJ/mol	Joback Method
hfus	47.06	kJ/mol	Joback Method
hvap	89.94	kJ/mol	Joback Method
log10ws	-6.66		Crippen Method
logp	5.921		Crippen Method
mcvol	324.980	ml/mol	McGowan Method
pc	1231.15	kPa	Joback Method
rinpol	2835.00		NIST Webbook
tb	946.05	K	Joback Method
tc	1166.77	K	Joback Method
tf	524.12	K	Joback Method
vc	1.232	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1085.02	J/mol×K	946.05	Joback Method
cpg	1151.25	J/mol×K	1129.98	Joback Method
cpg	1140.91	J/mol×K	1093.19	Joback Method
cpg	1129.18	J/mol×K	1056.41	Joback Method
cpg	1115.99	J/mol×K	1019.62	Joback Method
cpg	1101.29	J/mol×K	982.84	Joback Method
cpg	1160.25	J/mol×K	1166.77	Joback Method
dvisc	0.0000309	Pa×s	946.05	Joback Method
dvisc	0.0000413	Pa×s	875.73	Joback Method

dvisc	0.0000579	Pa×s	805.41	Joback Method
dvisc	0.0000868	Pa×s	735.09	Joback Method
dvisc	0.0001418	Pa×s	664.76	Joback Method
dvisc	0.0002599	Pa×s	594.44	Joback Method
dvisc	0.0005608	Pa×s	524.12	Joback Method

Sources

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=U416464&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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