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

Inchi: InChI=1S/C25H36O4/c1-2-3-19-28-24(26)17-11-6-12-18-25(27)29-23(22-15-9-5-10-16-2
InchiKey: PHWKJHKJOCBOOE-UHFFFAOYSA-N
Formula: C25H36O4
SMILES: CCCCOC(=O)CCCCCC(=O)OC(CC1C=CCCC1)c1ccccc1
Mol. weight [g/mol]: 400.55

Physical Properties

Property code	Value	Unit	Source
gf	-143.84	kJ/mol	Joback Method
hf	-705.58	kJ/mol	Joback Method
hfus	49.65	kJ/mol	Joback Method
hvap	92.17	kJ/mol	Joback Method
log10ws	-7.08		Crippen Method
logp	6.311		Crippen Method
mcvol	339.070	ml/mol	McGowan Method
pc	1152.22	kPa	Joback Method
rinpol	2932.00		NIST Webbook
rinpol	2932.00		NIST Webbook
tb	968.93	K	Joback Method
tc	1191.22	K	Joback Method
tf	535.39	K	Joback Method
vc	1.288	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1146.22	J/mol×K	968.93	Joback Method
cpg	1211.88	J/mol×K	1154.17	Joback Method
cpg	1201.71	J/mol×K	1117.12	Joback Method
cpg	1190.12	J/mol×K	1080.07	Joback Method
cpg	1177.05	J/mol×K	1043.03	Joback Method
cpg	1162.44	J/mol×K	1005.98	Joback Method
cpg	1220.69	J/mol×K	1191.22	Joback Method
dvisc	0.0000266	Pa×s	968.93	Joback Method

dvisc	0.0000355	Pa×s	896.67	Joback Method
dvisc	0.0000500	Pa×s	824.42	Joback Method
dvisc	0.0000752	Pa×s	752.16	Joback Method
dvisc	0.0001234	Pa×s	679.90	Joback Method
dvisc	0.0002276	Pa×s	607.65	Joback Method
dvisc	0.0004953	Pa×s	535.39	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416466&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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