1,2-Cyclohexanedicarboxylic acid, isohexyl 3-phenylpropyl ester

Inchi: InChI=1S/C23H34O4/c1-18(2)10-8-16-26-22(24)20-14-6-7-15-21(20)23(25)27-17-9-13-1

InchiKey: FGNSYVCEACGATI-UHFFFAOYSA-N

Formula: C23H34O4

SMILES: CC(C)CCCOC(=O)C1CCCCC1C(=O)OCCCc1ccccc1

Mol. weight [g/mol]: 374.51

Physical Properties

Property code	Value	Unit	Source
gf	-198.35	kJ/mol	Joback Method
hf	-742.42	kJ/mol	Joback Method
hfus	44.32	kJ/mol	Joback Method
hvap	87.11	kJ/mol	Joback Method
log10ws	-5.45		Crippen Method
logp	4.948		Crippen Method
mcvol	315.190	ml/mol	McGowan Method
pc	1254.81	kPa	Joback Method
rinpol	2700.00		NIST Webbook
tb	919.34	K	Joback Method
tc	1138.16	K	Joback Method
tf	507.85	K	Joback Method
vc	1.190	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1058.70	J/mol×K	919.34	Joback Method
cpg	1075.98	J/mol×K	955.81	Joback Method
cpg	1091.61	J/mol×K	992.28	Joback Method
cpg	1105.61	J/mol×K	1028.75	Joback Method
cpg	1118.05	J/mol×K	1065.22	Joback Method
cpg	1128.95	J/mol×K	1101.69	Joback Method
cpg	1138.35	J/mol×K	1138.16	Joback Method
dvisc	0.0007045	Pa×s	507.85	Joback Method
dvisc	0.0003360	Pa×s	576.43	Joback Method

dvisc	0.0001876	Pa×s	645.01	Joback Method
dvisc	0.0001171	Pa×s	713.60	Joback Method
dvisc	0.0000794	Pa×s	782.18	Joback Method
dvisc	0.0000573	Pa×s	850.76	Joback Method
dvisc	0.0000435	Pa×s	919.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339497&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