1,2-Cyclohexanedicarboxylic acid, 3,5-dimethylcyclohexyl isohexyl ester

Inchi: InChI=1S/C22H38O4/c1-15(2)8-7-11-25-21(23)19-9-5-6-10-20(19)22(24)26-18-13-16(3)12-17(4)14-18/h15-20H,5-14H2,1-4H3

InchiKey: NJNRLUXBESLGST-UHFFFAOYSA-N

Formula: C22H38O4

SMILES: CC(C)CCCOC(=O)C1CCCCC1C(=O)OC1CC(C)CC(C)C1

Mol. weight [g/mol]: 366.53

Physical Properties

Property code	Value	Unit	Source
gf	-310.15	kJ/mol	Joback Method
hf	-944.67	kJ/mol	Joback Method
hfus	41.67	kJ/mol	Joback Method
hvap	82.42	kJ/mol	Joback Method
log10ws	-5.45		Crippen Method
logp	5.140		Crippen Method
mcvol	314.000	ml/mol	McGowan Method
pc	1173.63	kPa	Joback Method
rinpol	2418.00		NIST Webbook
rinpol	2418.00		NIST Webbook
tb	879.99	K	Joback Method
tc	1094.28	K	Joback Method
tf	469.06	K	Joback Method
vc	1.173	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1097.90	J/mol×K	879.99	Joback Method
cpg	1118.66	J/mol×K	915.71	Joback Method
cpg	1137.49	J/mol×K	951.42	Joback Method
cpg	1154.40	J/mol×K	987.14	Joback Method
cpg	1169.42	J/mol×K	1022.85	Joback Method
cpg	1182.56	J/mol×K	1058.57	Joback Method
cpg	1193.84	J/mol×K	1094.28	Joback Method
dvisc	0.0012161	Pa×s	469.06	Joback Method

dvisc	0.0005902	Pa×s	537.55	Joback Method
dvisc	0.0003372	Pa×s	606.04	Joback Method
dvisc	0.0002159	Pa×s	674.52	Joback Method
dvisc	0.0001501	Pa×s	743.01	Joback Method
dvisc	0.0001109	Pa×s	811.50	Joback Method
dvisc	0.0000859	Pa×s	879.99	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=U339849&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