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

Inchi: InChI=1S/C22H38O4/c1-4-5-6-9-12-25-21(23)19-10-7-8-11-20(19)22(24)26-18-14-16(2)1

InchiKey: WEYNQVXJYNZXOX-UHFFFAOYSA-N

Formula: C22H38O4

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

Mol. weight [g/mol]: 366.53

Physical Properties

Property code	Value	Unit	Source
gf	-307.71	kJ/mol	Joback Method
hf	-939.39	kJ/mol	Joback Method
hfus	45.19	kJ/mol	Joback Method
hvap	82.81	kJ/mol	Joback Method
log10ws	-5.69		Crippen Method
logp	5.284		Crippen Method
mcvol	314.000	ml/mol	McGowan Method
pc	1167.22	kPa	Joback Method
rinpol	2467.00		NIST Webbook
rinpol	2467.00		NIST Webbook
tb	880.43	K	Joback Method
tc	1092.67	K	Joback Method
tf	484.06	K	Joback Method
vc	1.179	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1097.46	J/mol×K	880.43	Joback Method
cpg	1118.04	J/mol×K	915.80	Joback Method
cpg	1136.74	J/mol×K	951.18	Joback Method
cpg	1153.58	J/mol×K	986.55	Joback Method
cpg	1168.57	J/mol×K	1021.92	Joback Method
cpg	1181.72	J/mol×K	1057.30	Joback Method
cpg	1193.05	J/mol×K	1092.67	Joback Method
dvisc	0.0010786	Pa×s	484.06	Joback Method

dvisc	0.0005625	Pa×s	550.12	Joback Method
dvisc	0.0003373	Pa×s	616.18	Joback Method
dvisc	0.0002233	Pa×s	682.25	Joback Method
dvisc	0.0001590	Pa×s	748.31	Joback Method
dvisc	0.0001197	Pa×s	814.37	Joback Method
dvisc	0.0000940	Pa×s	880.43	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339850&Units=SI

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