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

Inchi: InChI=1S/C21H36O4/c1-4-5-8-11-24-20(22)18-9-6-7-10-19(18)21(23)25-17-13-15(2)12-1

InchiKey: CNSKQIPMGXCCKR-UHFFFAOYSA-N

Formula: C21H36O4

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

Mol. weight [g/mol]: 352.51

Physical Properties

Property code	Value	Unit	Source
gf	-316.13	kJ/mol	Joback Method
hf	-918.75	kJ/mol	Joback Method
hfus	42.60	kJ/mol	Joback Method
hvap	80.58	kJ/mol	Joback Method
log10ws	-5.27		Crippen Method
logp	4.894		Crippen Method
mcvol	299.910	ml/mol	McGowan Method
pc	1247.73	kPa	Joback Method
rinpol	2369.00		NIST Webbook
rinpol	2369.00		NIST Webbook
tb	857.55	K	Joback Method
tc	1070.02	K	Joback Method
tf	472.79	K	Joback Method
vc	1.123	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1035.08	J/mol×K	857.55	Joback Method
cpg	1055.95	J/mol×K	892.96	Joback Method
cpg	1074.98	J/mol×K	928.37	Joback Method
cpg	1092.18	J/mol×K	963.79	Joback Method
cpg	1107.58	J/mol×K	999.20	Joback Method
cpg	1121.17	J/mol×K	1034.61	Joback Method
cpg	1132.97	J/mol×K	1070.02	Joback Method
dvisc	0.0011802	Pa×s	472.79	Joback Method

dvisc	0.0006229	Pa×s	536.92	Joback Method
dvisc	0.0003768	Pa×s	601.04	Joback Method
dvisc	0.0002511	Pa×s	665.17	Joback Method
dvisc	0.0001797	Pa×s	729.30	Joback Method
dvisc	0.0001358	Pa×s	793.42	Joback Method
dvisc	0.0001070	Pa×s	857.55	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=U339848&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