1,2-Cyclohexanedicarboxylic acid, decyl 3-methylbut-2-yl ester

Inchi: InChI=1S/C23H42O4/c1-5-6-7-8-9-10-11-14-17-26-22(24)20-15-12-13-16-21(20)23(25)2

InchiKey: ZTZBBTWFEIKNJE-UHFFFAOYSA-N

Formula: C23H42O4

SMILES: CCCCCCCCCCOC(=O)C1CCCCC1C(=O)OC(C)C(C)C

Mol. weight [g/mol]: 382.58

Physical Properties

Property code	Value	Unit	Source
gf	-313.20	kJ/mol	Joback Method
hf	-984.23	kJ/mol	Joback Method
hfus	46.76	kJ/mol	Joback Method
hvap	84.45	kJ/mol	Joback Method
log10ws	-6.46		Crippen Method
logp	6.064		Crippen Method
mcvol	338.950	ml/mol	McGowan Method
pc	1010.37	kPa	Joback Method
rinpol	2538.00		NIST Webbook
rinpol	2538.00		NIST Webbook
tb	892.22	K	Joback Method
tc	1095.57	K	Joback Method
tf	466.43	K	Joback Method
vc	1.292	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1156.49	J/mol×K	892.22	Joback Method
cpg	1176.20	J/mol×K	926.11	Joback Method
cpg	1194.34	J/mol×K	960.00	Joback Method
cpg	1210.94	J/mol×K	993.90	Joback Method
cpg	1226.04	J/mol×K	1027.79	Joback Method
cpg	1239.65	J/mol×K	1061.68	Joback Method
cpg	1251.81	J/mol×K	1095.57	Joback Method
dvisc	0.0009832	Pa×s	466.43	Joback Method

dvisc	0.0004013	Pa×s	537.39	Joback Method
dvisc	0.0002019	Pa×s	608.36	Joback Method
dvisc	0.0001173	Pa×s	679.33	Joback Method
dvisc	0.0000755	Pa×s	750.29	Joback Method
dvisc	0.0000524	Pa×s	821.26	Joback Method
dvisc	0.0000386	Pa×s	892.22	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=U339563&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