1,2-Cyclohexanedicarboxylic acid, dodecyl isopropyl ester

Inchi: InChI=1S/C23H42O4/c1-4-5-6-7-8-9-10-11-12-15-18-26-22(24)20-16-13-14-17-21(20)23

InchiKey: MFYFEENVHQLNLN-UHFFFAOYSA-N

Formula: C23H42O4

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

Mol. weight [g/mol]: 382.58

Physical Properties

Property code	Value	Unit	Source
gf	-310.76	kJ/mol	Joback Method
hf	-978.95	kJ/mol	Joback Method
hfus	50.28	kJ/mol	Joback Method
hvap	84.84	kJ/mol	Joback Method
log10ws	-6.70		Crippen Method
logp	6.209		Crippen Method
mcvol	338.950	ml/mol	McGowan Method
pc	1005.26	kPa	Joback Method
rinpol	2675.00		NIST Webbook
rinpol	2675.00		NIST Webbook
tb	892.66	K	Joback Method
tc	1095.22	K	Joback Method
tf	481.43	K	Joback Method
vc	1.298	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1156.06	J/mol×K	892.66	Joback Method
cpg	1239.17	J/mol×K	1061.46	Joback Method
cpg	1225.52	J/mol×K	1027.70	Joback Method
cpg	1210.41	J/mol×K	993.94	Joback Method
cpg	1193.82	J/mol×K	960.18	Joback Method
cpg	1175.71	J/mol×K	926.42	Joback Method
cpg	1251.39	J/mol×K	1095.22	Joback Method
dvisc	0.0000422	Pa×s	892.66	Joback Method

dvisc	0.0000565	Pa×s	824.12	Joback Method
dvisc	0.0000797	Pa×s	755.58	Joback Method
dvisc	0.0001204	Pa×s	687.04	Joback Method
dvisc	0.0001994	Pa×s	618.51	Joback Method
dvisc	0.0003744	Pa×s	549.97	Joback Method
dvisc	0.0008412	Pa×s	481.43	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339646&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