1,2-Cyclohexanedicarboxylic acid, hexyl methyl ester

Inchi: InChI=1S/C15H26O4/c1-3-4-5-8-11-19-15(17)13-10-7-6-9-12(13)14(16)18-2/h12-13H,3-1

InchiKey: COXGMKRNKWLBNQ-UHFFFAOYSA-N

Formula: C15H26O4

SMILES: CCCCCCOC(=O)C1CCCCC1C(=O)OC

Mol. weight [g/mol]: 270.36

Physical Properties

Property code	Value	Unit	Source
gf	-375.68	kJ/mol	Joback Method
hf	-808.55	kJ/mol	Joback Method
hfus	33.09	kJ/mol	Joback Method
hvap	67.42	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	3.089		Crippen Method
mcvol	226.230	ml/mol	McGowan Method
pc	1744.82	kPa	Joback Method
rinpol	1873.00		NIST Webbook
tb	710.06	K	Joback Method
tc	907.67	K	Joback Method
tf	406.27	K	Joback Method
vc	0.856	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	674.22	J/mol×K	710.06	Joback Method
cpg	692.80	J/mol×K	743.00	Joback Method
cpg	710.26	J/mol×K	775.93	Joback Method
cpg	726.62	J/mol×K	808.87	Joback Method
cpg	741.88	J/mol×K	841.80	Joback Method
cpg	756.04	J/mol×K	874.74	Joback Method
cpg	769.11	J/mol×K	907.67	Joback Method
dvisc	0.0015847	Pa×s	406.27	Joback Method
dvisc	0.0008379	Pa×s	456.90	Joback Method

dvisc	0.0005032	Pa×s	507.53	Joback Method
dvisc	0.0003314	Pa×s	558.16	Joback Method
dvisc	0.0002340	Pa×s	608.80	Joback Method
dvisc	0.0001743	Pa×s	659.43	Joback Method
dvisc	0.0001354	Pa×s	710.06	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=U339653&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