Cyclohexanecarboxylic acid, 4-methoxy-, hexyl ester

Inchi: InChI=1S/C14H26O3/c1-3-4-5-6-11-17-14(15)12-7-9-13(16-2)10-8-12/h12-13H,3-11H2,1

InchiKey: OZPMVNPIQAEKEQ-UHFFFAOYSA-N

Formula: C14H26O3

SMILES: CCCCCCOC(=O)C1CCC(OC)CC1

Mol. weight [g/mol]: 242.35

Physical Properties

Property code	Value	Unit	Source
gf	-255.18	kJ/mol	Joback Method
hf	-675.33	kJ/mol	Joback Method
hfus	28.90	kJ/mol	Joback Method
hvap	58.44	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	3.315		Crippen Method
mcvol	210.570	ml/mol	McGowan Method
pc	1793.94	kPa	Joback Method
rinpol	1744.00		NIST Webbook
rinpol	1744.00		NIST Webbook
tb	633.31	K	Joback Method
tc	826.00	K	Joback Method
tf	345.07	K	Joback Method
vc	0.793	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	591.32	J/mol×K	633.31	Joback Method
cpg	611.20	J/mol×K	665.42	Joback Method
cpg	630.08	J/mol×K	697.54	Joback Method
cpg	647.97	J/mol×K	729.65	Joback Method
cpg	664.85	J/mol×K	761.77	Joback Method
cpg	680.74	J/mol×K	793.88	Joback Method
cpg	695.65	J/mol×K	826.00	Joback Method
dvisc	0.0020843	Pa×s	345.07	Joback Method

dvisc	0.0010281	Pa×s	393.11	Joback Method
dvisc	0.0005915	Pa×s	441.15	Joback Method
dvisc	0.0003793	Pa×s	489.19	Joback Method
dvisc	0.0002634	Pa×s	537.23	Joback Method
dvisc	0.0001942	Pa×s	585.27	Joback Method
dvisc	0.0001499	Pa×s	633.31	Joback Method

Sources

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=U406194&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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