1,2-Cyclohexanedicarboxylic acid, hexyl 2-methoxyethyl ester

Inchi: InChI=1S/C17H30O5/c1-3-4-5-8-11-21-16(18)14-9-6-7-10-15(14)17(19)22-13-12-20-2/h1

InchiKey: ATAQZNKQFNFBLW-UHFFFAOYSA-N

Formula: C17H30O5

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

Mol. weight [g/mol]: 314.42

Physical Properties

Property code	Value	Unit	Source
gf	-463.84	kJ/mol	Joback Method
hf	-982.05	kJ/mol	Joback Method
hfus	39.45	kJ/mol	Joback Method
hvap	74.28	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	3.106		Crippen Method
mcvol	260.280	ml/mol	McGowan Method
pc	1475.88	kPa	Joback Method
rinpol	2234.00		NIST Webbook
rinpol	2234.00		NIST Webbook
tb	778.24	K	Joback Method
tc	973.30	K	Joback Method
tf	451.04	K	Joback Method
vc	0.986	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	820.53	J/mol×K	778.24	Joback Method
cpg	900.26	J/mol×K	940.79	Joback Method
cpg	886.78	J/mol×K	908.28	Joback Method
cpg	872.06	J/mol×K	875.77	Joback Method
cpg	856.11	J/mol×K	843.26	Joback Method
cpg	838.93	J/mol×K	810.75	Joback Method
cpg	912.51	J/mol×K	973.30	Joback Method
dvisc	0.0000803	Pa×s	778.24	Joback Method

dvisc	0.0001037	Pa×s	723.71	Joback Method
dvisc	0.0001398	Pa×s	669.17	Joback Method
dvisc	0.0001985	Pa×s	614.64	Joback Method
dvisc	0.0003019	Pa×s	560.11	Joback Method
dvisc	0.0005025	Pa×s	505.57	Joback Method
dvisc	0.0009463	Pa×s	451.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U340028&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