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

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

InchiKey: ZFUVEGUFOGCMEN-UHFFFAOYSA-N

Formula: C17H30O5

SMILES: COCCOC(=O)C1CCCCC1C(=O)OCCCC(C)C

Mol. weight [g/mol]: 314.42

Physical Properties

Property code	Value	Unit	Source
gf	-466.28	kJ/mol	Joback Method
hf	-987.33	kJ/mol	Joback Method
hfus	35.93	kJ/mol	Joback Method
hvap	73.89	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	2.962		Crippen Method
mcvol	260.280	ml/mol	McGowan Method
pc	1485.00	kPa	Joback Method
rinpol	2089.00		NIST Webbook
rinpol	2089.00		NIST Webbook
tb	777.80	K	Joback Method
tc	975.15	K	Joback Method
tf	436.04	K	Joback Method
vc	0.980	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	821.02	J/mol×K	777.80	Joback Method
cpg	901.48	J/mol×K	942.26	Joback Method
cpg	887.93	J/mol×K	909.36	Joback Method
cpg	873.10	J/mol×K	876.47	Joback Method
cpg	857.01	J/mol×K	843.58	Joback Method
cpg	839.65	J/mol×K	810.69	Joback Method
cpg	913.75	J/mol×K	975.15	Joback Method
dvisc	0.0000739	Pa×s	777.80	Joback Method

dvisc	0.0000970	Pa×s	720.84	Joback Method
dvisc	0.0001335	Pa×s	663.88	Joback Method
dvisc	0.0001952	Pa×s	606.92	Joback Method
dvisc	0.0003086	Pa×s	549.96	Joback Method
dvisc	0.0005423	Pa×s	493.00	Joback Method
dvisc	0.0011045	Pa×s	436.04	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=U340027&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