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

Inchi: InChI=1S/C18H32O5/c1-3-4-5-6-9-12-22-17(19)15-10-7-8-11-16(15)18(20)23-14-13-21-2

InchiKey: REFRBEIGSXVJAQ-UHFFFAOYSA-N

Formula: C18H32O5

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

Mol. weight [g/mol]: 328.44

Physical Properties

Property code	Value	Unit	Source
gf	-455.42	kJ/mol	Joback Method
hf	-1002.69	kJ/mol	Joback Method
hfus	42.04	kJ/mol	Joback Method
hvap	76.50	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	3.496		Crippen Method
mcvol	274.370	ml/mol	McGowan Method
pc	1372.76	kPa	Joback Method
rinpol	2226.00		NIST Webbook
rinpol	2226.00		NIST Webbook
tb	801.12	K	Joback Method
tc	996.18	K	Joback Method
tf	462.31	K	Joback Method
vc	1.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	880.01	J/mol×K	801.12	Joback Method
cpg	898.52	J/mol×K	833.63	Joback Method
cpg	915.76	J/mol×K	866.14	Joback Method
cpg	931.71	J/mol×K	898.65	Joback Method
cpg	946.39	J/mol×K	931.16	Joback Method
cpg	959.78	J/mol×K	963.67	Joback Method
cpg	971.90	J/mol×K	996.18	Joback Method
dvisc	0.0008608	Pa×s	462.31	Joback Method

dvisc	0.0004515	Pa×s	518.78	Joback Method
dvisc	0.0002688	Pa×s	575.25	Joback Method
dvisc	0.0001756	Pa×s	631.72	Joback Method
dvisc	0.0001230	Pa×s	688.18	Joback Method
dvisc	0.0000909	Pa×s	744.65	Joback Method
dvisc	0.0000702	Pa×s	801.12	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=U340029&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