1,2-Cyclohexanedicarboxylic acid, cyclohexylmethyl ethyl ester

Inchi: InChI=1S/C17H28O4/c1-2-20-16(18)14-10-6-7-11-15(14)17(19)21-12-13-8-4-3-5-9-13/h1

InchiKey: MNGOTHKTFMBVNF-UHFFFAOYSA-N

Formula: C17H28O4

SMILES: CCOC(=O)C1CCCCC1C(=O)OCC1CCCCC1

Mol. weight [g/mol]: 296.40

Physical Properties

Property code	Value	Unit	Source
gf	-334.39	kJ/mol	Joback Method
hf	-795.51	kJ/mol	Joback Method
hfus	30.10	kJ/mol	Joback Method
hvap	72.30	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	3.479		Crippen Method
mcvol	243.550	ml/mol	McGowan Method
pc	1763.93	kPa	Joback Method
rinpol	2113.00		NIST Webbook
rinpol	2113.00		NIST Webbook
tb	775.37	K	Joback Method
tc	995.32	K	Joback Method
tf	436.19	K	Joback Method
vc	0.900	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	785.99	J/mol×K	775.37	Joback Method
cpg	873.95	J/mol×K	958.66	Joback Method
cpg	859.60	J/mol×K	922.00	Joback Method
cpg	843.65	J/mol×K	885.35	Joback Method
cpg	826.07	J/mol×K	848.69	Joback Method
cpg	806.86	J/mol×K	812.03	Joback Method
cpg	886.71	J/mol×K	995.32	Joback Method
dvisc	0.0001103	Pa×s	775.37	Joback Method

dvisc	0.0001443	Pa×s	718.84	Joback Method
dvisc	0.0001976	Pa×s	662.31	Joback Method
dvisc	0.0002870	Pa×s	605.78	Joback Method
dvisc	0.0004501	Pa×s	549.25	Joback Method
dvisc	0.0007826	Pa×s	492.72	Joback Method
dvisc	0.0015707	Pa×s	436.19	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339736&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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