1,2-Cyclohexanedicarboxylic acid, cyclohexyl isobutyl ester

Inchi: InChI=1S/C18H30O4/c1-13(2)12-21-17(19)15-10-6-7-11-16(15)18(20)22-14-8-4-3-5-9-14

InchiKey: IDGQDODXHJFNKL-UHFFFAOYSA-N

Formula: C18H30O4

SMILES: CC(C)COC(=O)C1CCCCC1C(=O)OC1CCCCC1

Mol. weight [g/mol]: 310.43

Physical Properties

Property code	Value	Unit	Source
gf	-328.41	kJ/mol	Joback Method
hf	-821.43	kJ/mol	Joback Method
hfus	29.17	kJ/mol	Joback Method
hvap	74.14	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	3.868		Crippen Method
mcvol	257.640	ml/mol	McGowan Method
pc	1640.43	kPa	Joback Method
rinpol	2139.00		NIST Webbook
rinpol	2139.00		NIST Webbook
tb	797.81	K	Joback Method
tc	1018.41	K	Joback Method
tf	432.46	K	Joback Method
vc	0.951	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	846.01	J/mol×K	797.81	Joback Method
cpg	933.89	J/mol×K	981.64	Joback Method
cpg	919.70	J/mol×K	944.87	Joback Method
cpg	903.84	J/mol×K	908.11	Joback Method
cpg	886.28	J/mol×K	871.34	Joback Method
cpg	867.01	J/mol×K	834.58	Joback Method
cpg	946.42	J/mol×K	1018.41	Joback Method
dvisc	0.0000887	Pa×s	797.81	Joback Method

dvisc	0.0001184	Pa×s	736.92	Joback Method
dvisc	0.0001663	Pa×s	676.03	Joback Method
dvisc	0.0002498	Pa×s	615.13	Joback Method
dvisc	0.0004105	Pa×s	554.24	Joback Method
dvisc	0.0007624	Pa×s	493.35	Joback Method
dvisc	0.0016860	Pa×s	432.46	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339759&Units=SI

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