1,2-Cyclohexanedicarboxylic acid, isobutyl pentyl ester

Inchi: InChI=1S/C17H30O4/c1-4-5-8-11-20-16(18)14-9-6-7-10-15(14)17(19)21-12-13(2)3/h13-1
InchiKey: OLYHQZVEXBYJFM-UHFFFAOYSA-N
Formula: C17H30O4
SMILES: CCCCCOC(=O)C1CCCCC1C(=O)OCC(C)C
Mol. weight [g/mol]: 298.42

Physical Properties

Property code	Value	Unit	Source
gf	-361.28	kJ/mol	Joback Method
hf	-855.11	kJ/mol	Joback Method
hfus	34.74	kJ/mol	Joback Method
hvap	71.48	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.725		Crippen Method
mcvol	254.410	ml/mol	McGowan Method
pc	1504.65	kPa	Joback Method
rinpol	1978.00		NIST Webbook
rinpol	1978.00		NIST Webbook
tb	755.38	K	Joback Method
tc	952.93	K	Joback Method
tf	413.81	K	Joback Method
vc	0.962	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	790.12	J/mol×K	755.38	Joback Method
cpg	809.29	J/mol×K	788.31	Joback Method
cpg	827.24	J/mol×K	821.23	Joback Method
cpg	843.97	J/mol×K	854.16	Joback Method
cpg	859.49	J/mol×K	887.08	Joback Method
cpg	873.82	J/mol×K	920.01	Joback Method
cpg	886.95	J/mol×K	952.93	Joback Method
dvisc	0.0015981	Pa×s	413.81	Joback Method

dvisc	0.0007558	Pa×s	470.74	Joback Method
dvisc	0.0004201	Pa×s	527.67	Joback Method
dvisc	0.0002618	Pa×s	584.60	Joback Method
dvisc	0.0001775	Pa×s	641.52	Joback Method
dvisc	0.0001282	Pa×s	698.45	Joback Method
dvisc	0.0000972	Pa×s	755.38	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=U339425&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