1,2-Cyclohexanedicarboxylic acid, isohexyl 3-methylbut-2-yl ester

Inchi: InChI=1S/C19H34O4/c1-13(2)9-8-12-22-18(20)16-10-6-7-11-17(16)19(21)23-15(5)14(3)4

InchiKey: WMVCZLYJRCESGN-UHFFFAOYSA-N

Formula: C19H34O4

SMILES: CC(C)CCCOC(=O)C1CCCCC1C(=O)OC(C)C(C)C

Mol. weight [g/mol]: 326.47

Physical Properties

Property code	Value	Unit	Source
gf	-349.32	kJ/mol	Joback Method
hf	-906.95	kJ/mol	Joback Method
hfus	32.88	kJ/mol	Joback Method
hvap	75.16	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	4.360		Crippen Method
mcvol	282.590	ml/mol	McGowan Method
pc	1318.48	kPa	Joback Method
rinpol	2080.00		NIST Webbook
rinpol	2080.00		NIST Webbook
tb	800.26	K	Joback Method
tc	1001.13	K	Joback Method
tf	406.35	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	910.20	J/mol×K	800.26	Joback Method
cpg	929.97	J/mol×K	833.74	Joback Method
cpg	948.36	J/mol×K	867.22	Joback Method
cpg	965.38	J/mol×K	900.70	Joback Method
cpg	981.04	J/mol×K	934.17	Joback Method
cpg	995.36	J/mol×K	967.65	Joback Method
cpg	1008.36	J/mol×K	1001.13	Joback Method
dvisc	0.0019269	Pa×s	406.35	Joback Method

dvisc	0.0007324	Pa×s	472.00	Joback Method
dvisc	0.0003526	Pa×s	537.65	Joback Method
dvisc	0.0001990	Pa×s	603.31	Joback Method
dvisc	0.0001256	Pa×s	668.96	Joback Method
dvisc	0.0000861	Pa×s	734.61	Joback Method
dvisc	0.0000628	Pa×s	800.26	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=U339559&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