1,2-Cyclohexanedicarboxylic acid, isohexyl 2-methylcyclohexyl ester

Inchi: InChI=1S/C21H36O4/c1-15(2)9-8-14-24-20(22)17-11-5-6-12-18(17)21(23)25-19-13-7-4-1

InchiKey: SWXNIJYBJZYDKA-UHFFFAOYSA-N

Formula: C21H36O4

SMILES: CC(C)CCCOC(=O)C1CCCCC1C(=O)OC1CCCCC1C

Mol. weight [g/mol]: 352.51

Physical Properties

Property code	Value	Unit	Source
gf	-310.86	kJ/mol	Joback Method
hf	-903.69	kJ/mol	Joback Method
hfus	38.01	kJ/mol	Joback Method
hvap	80.50	kJ/mol	Joback Method
log10ws	-5.27		Crippen Method
logp	4.894		Crippen Method
mcvol	299.910	ml/mol	McGowan Method
pc	1284.67	kPa	Joback Method
rinpol	2378.00		NIST Webbook
tb	861.78	K	Joback Method
tc	1076.90	K	Joback Method
tf	462.03	K	Joback Method
vc	1.117	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1032.18	J/mol×K	861.78	Joback Method
cpg	1052.84	J/mol×K	897.63	Joback Method
cpg	1071.67	J/mol×K	933.49	Joback Method
cpg	1088.67	J/mol×K	969.34	Joback Method
cpg	1103.87	J/mol×K	1005.19	Joback Method
cpg	1117.30	J/mol×K	1041.05	Joback Method
cpg	1128.96	J/mol×K	1076.90	Joback Method
dvisc	0.0012780	Pa×s	462.03	Joback Method
dvisc	0.0005929	Pa×s	528.65	Joback Method

dvisc	0.0003267	Pa×s	595.28	Joback Method
dvisc	0.0002030	Pa×s	661.90	Joback Method
dvisc	0.0001376	Pa×s	728.53	Joback Method
dvisc	0.0000995	Pa×s	795.15	Joback Method
dvisc	0.0000757	Pa×s	861.78	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=U339879&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