

1,2-Cyclohexanedicarboxylic acid, isobutyl methyl ester

Inchi:	InChI=1S/C13H22O4/c1-9(2)8-17-13(15)11-7-5-4-6-10(11)12(14)16-3/h9-11H,4-8H2,1-3
InchiKey:	BTHYGKGSTPCTCD-UHFFFAOYSA-N
Formula:	C13H22O4
SMILES:	COC(=O)C1CCCCC1C(=O)OCC(C)C
Mol. weight [g/mol]:	242.31

Physical Properties

Property code	Value	Unit	Source
gf	-394.96	kJ/mol	Joback Method
hf	-772.55	kJ/mol	Joback Method
hfus	24.38	kJ/mol	Joback Method
hvap	62.58	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	2.165		Crippen Method
mcvol	198.050	ml/mol	McGowan Method
pc	2077.43	kPa	Joback Method
rinpol	1627.00		NIST Webbook
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tb	663.86	K	Joback Method
tc	869.51	K	Joback Method
tf	368.73	K	Joback Method
vc	0.738	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	563.65	J/molxK	663.86	Joback Method
cpg	582.05	J/molxK	698.13	Joback Method
cpg	599.36	J/molxK	732.41	Joback Method
cpg	615.59	J/molxK	766.68	Joback Method
cpg	630.75	J/molxK	800.96	Joback Method
cpg	644.82	J/molxK	835.23	Joback Method
cpg	657.80	J/molxK	869.51	Joback Method
dvisc	0.0022079	Paxs	368.73	Joback Method

dvisc	0.0010990	Paxs	417.92	Joback Method
dvisc	0.0006337	Paxs	467.11	Joback Method
dvisc	0.0004058	Paxs	516.30	Joback Method
dvisc	0.0002808	Paxs	565.48	Joback Method
dvisc	0.0002061	Paxs	614.67	Joback Method
dvisc	0.0001584	Paxs	663.86	Joback Method

Sources

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=U339650&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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

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