

cis-3-Methyl-4-cyclohexene-1,2-dicarboxylic acid

Inchi:	InChI=1S/C9H12O4/c1-5-3-2-4-6(8(10)11)7(5)9(12)13/h2-3,5-7H,4H2,1H3,(H,10,11)(H,1
InchiKey:	ZPRXNOLDXHXIQ-UHFFFAOYSA-N
Formula:	C9H12O4
SMILES:	CC1C=CCC(C(=O)O)C1C(=O)O
Mol. weight [g/mol]:	184.19
CAS:	40469-16-7

Physical Properties

Property code	Value	Unit	Source
gf	-467.59	kJ/mol	Joback Method
hf	-687.29	kJ/mol	Joback Method
hfus	25.64	kJ/mol	Joback Method
hvap	82.58	kJ/mol	Joback Method
log10ws	-0.81		Crippen Method
logp	0.984		Crippen Method
mcvol	137.390	ml/mol	McGowan Method
pc	3920.94	kPa	Joback Method
tb	706.79	K	Joback Method
tc	901.55	K	Joback Method
tf	412.35	K	Joback Method
vc	0.506	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.02	J/molxK	706.79	Joback Method
cpg	405.54	J/molxK	739.25	Joback Method
cpg	415.37	J/molxK	771.71	Joback Method
cpg	424.53	J/molxK	804.17	Joback Method
cpg	433.02	J/molxK	836.63	Joback Method
cpg	440.87	J/molxK	869.09	Joback Method
cpg	448.07	J/molxK	901.55	Joback Method
dvisc	0.0031583	Paxs	412.35	Joback Method
dvisc	0.0009587	Paxs	461.42	Joback Method

dvisc	0.0003660	Paxs	510.50	Joback Method
dvisc	0.0001654	Paxs	559.57	Joback Method
dvisc	0.0000850	Paxs	608.64	Joback Method
dvisc	0.0000482	Paxs	657.72	Joback Method
dvisc	0.0000296	Paxs	706.79	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=C40469167&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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