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: ZPRXNOLDOXHXIQ-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/mol×K	706.79	Joback Method
cpg	440.87	J/mol×K	869.09	Joback Method
cpg	433.02	J/mol×K	836.63	Joback Method
cpg	424.53	J/mol×K	804.17	Joback Method
cpg	415.37	J/mol×K	771.71	Joback Method
cpg	405.54	J/mol×K	739.25	Joback Method
cpg	448.07	J/mol×K	901.55	Joback Method
dvisc	0.0000296	Pa×s	706.79	Joback Method
dvisc	0.0000482	Pa×s	657.72	Joback Method

dvisc	0.0000850	Pa×s	608.64	Joback Method
dvisc	0.0001654	Pa×s	559.57	Joback Method
dvisc	0.0003660	Pa×s	510.50	Joback Method
dvisc	0.0009587	Pa×s	461.42	Joback Method
dvisc	0.0031583	Pa×s	412.35	Joback Method

Sources

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/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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