1,2-Cyclohexanedicarboxylic acid, 4-methyl, dimethyl ester

Inchi: InChI=1S/C11H18O4/c1-7-4-5-8(10(12)14-2)9(6-7)11(13)15-3/h7-9H,4-6H2,1-3H3
InchiKey: GADRQTDSMCWRTB-UHFFFAOYSA-N
Formula: C11H18O4
SMILES: COC(=O)C1CCC(C)CC1C(=O)OC
Mol. weight [g/mol]: 214.26

Physical Properties

Property code	Value	Unit	Source
gf	-417.07	kJ/mol	Joback Method
hf	-746.33	kJ/mol	Joback Method
hfus	23.80	kJ/mol	Joback Method
hvap	58.20	kJ/mol	Joback Method
log10ws	-1.32		Crippen Method
logp	1.385		Crippen Method
mcvol	169.870	ml/mol	McGowan Method
pc	2395.87	kPa	Joback Method
rinpol	1427.00		NIST Webbook
rinpol	1403.00		NIST Webbook
rinpol	1410.00		NIST Webbook
rinpol	1418.00		NIST Webbook
tb	613.87	K	Joback Method
tc	821.66	K	Joback Method
tf	356.95	K	Joback Method
vc	0.630	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	458.97	J/mol×K	613.87	Joback Method
cpg	476.63	J/mol×K	648.50	Joback Method
cpg	493.34	J/mol×K	683.13	Joback Method
cpg	509.10	J/mol×K	717.76	Joback Method
cpg	523.89	J/mol×K	752.40	Joback Method
cpg	537.71	J/mol×K	787.03	Joback Method

cpg	550.52	J/mol×K	821.66	Joback Method
dvisc	0.0018188	Pa×s	356.95	Joback Method
dvisc	0.0010882	Pa×s	399.77	Joback Method
dvisc	0.0007191	Pa×s	442.59	Joback Method
dvisc	0.0005113	Pa×s	485.41	Joback Method
dvisc	0.0003842	Pa×s	528.23	Joback Method
dvisc	0.0003013	Pa×s	571.05	Joback Method
dvisc	0.0002444	Pa×s	613.87	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R33886&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
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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