

1,2-CYCLOPENTANEDICARBOXYLIC ACID, DIMETHYL ESTER

Inchi: InChI=1S/C9H14O4/c1-12-8(10)6-4-3-5-7(6)9(11)13-2/h6-7H,3-5H2,1-2H3
InchiKey: XFLSEYYPOYRKKC-UHFFFAOYSA-N
Formula: C9H14O4
SMILES: COC(=O)C1CCCC1C(=O)OC
Mol. weight [g/mol]: 186.21

Physical Properties

Property code	Value	Unit	Source
chl	-4676.50	kJ/mol	NIST Webbook
hf	-760.92	kJ/mol	Cheméo Relay (1.0)
hfus	19.65	kJ/mol	Joback Method
hvap	71.85	kJ/mol	Cheméo Relay (1.0)
logp	0.749		Crippen Method
mcvol	141.690	ml/mol	McGowan Method
tb	494.27	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.51	J/mol×K	568.51	Joback Method
cpg	435.24	J/mol×K	776.09	Joback Method
cpg	424.04	J/mol×K	741.49	Joback Method
cpg	412.07	J/mol×K	706.90	Joback Method
cpg	399.32	J/mol×K	672.30	Joback Method
cpg	385.81	J/mol×K	637.70	Joback Method
cpg	371.53	J/mol×K	603.11	Joback Method
dvisc	0.0006386	Pa×s	455.34	Joback Method
dvisc	0.0003232	Pa×s	568.51	Joback Method
dvisc	0.0003927	Pa×s	530.79	Joback Method
dvisc	0.0004915	Pa×s	493.06	Joback Method
dvisc	0.0019796	Pa×s	342.17	Joback Method
dvisc	0.0008698	Pa×s	417.62	Joback Method
dvisc	0.0012597	Pa×s	379.89	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C68252175&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature

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