

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
CAS:	68252-17-5

Physical Properties

Property code	Value	Unit	Source
chl	-4676.50	kJ/mol	NIST Webbook
gf	-414.10	kJ/mol	Joback Method
hf	-678.55	kJ/mol	Joback Method
hfus	19.65	kJ/mol	Joback Method
hvap	53.89	kJ/mol	Joback Method
log10ws	-0.73		Crippen Method
logp	0.749		Crippen Method
mcvol	141.690	ml/mol	McGowan Method
pc	2944.08	kPa	Joback Method
tb	568.51	K	Joback Method
tc	776.09	K	Joback Method
tf	342.17	K	Joback Method
vc	0.527	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.51	J/molxK	568.51	Joback Method
cpg	371.53	J/molxK	603.11	Joback Method
cpg	385.81	J/molxK	637.70	Joback Method
cpg	399.32	J/molxK	672.30	Joback Method
cpg	412.07	J/molxK	706.90	Joback Method
cpg	424.04	J/molxK	741.49	Joback Method
cpg	435.24	J/molxK	776.09	Joback Method
dvisc	0.0019796	Paxs	342.17	Joback Method

dvisc	0.0012597	Paxs	379.89	Joback Method
dvisc	0.0008698	Paxs	417.62	Joback Method
dvisc	0.0006386	Paxs	455.34	Joback Method
dvisc	0.0004915	Paxs	493.06	Joback Method
dvisc	0.0003927	Paxs	530.79	Joback Method
dvisc	0.0003232	Paxs	568.51	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=C68252175&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
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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