1,2-Cyclobutanedicarboxylic acid, dimethyl ester

Other names: Dimethyl cyclobutane-1,2-dicarboxylate
Inchi: InChI=1S/C8H12O4/c1-11-7(9)5-3-4-6(5)8(10)12-2/h5-6H,3-4H2,1-2H3
InchiKey: WEPHXFVXUXMCLE-UHFFFAOYSA-N
Formula: C8H12O4
SMILES: COC(=O)C1CCC1C(=O)OC
Mol. weight [g/mol]: 172.18
CAS: 3396-20-1

Physical Properties

Property code	Value	Unit	Source
chl	-4119.00	kJ/mol	NIST Webbook
gf	-410.42	kJ/mol	Joback Method
hf	-651.75	kJ/mol	Joback Method
hfus	19.16	kJ/mol	Joback Method
hvap	51.49	kJ/mol	Joback Method
log10ws	-0.31		Crippen Method
logp	0.359		Crippen Method
mcvol	127.600	ml/mol	McGowan Method
pc	3184.73	kPa	Joback Method
tb	541.36	K	Joback Method
tc	745.03	K	Joback Method
tf	334.42	K	Joback Method
vc	0.479	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	309.19	J/mol×K	541.36	Joback Method
cpg	369.38	J/mol×K	711.09	Joback Method
cpg	358.61	J/mol×K	677.14	Joback Method
cpg	347.20	J/mol×K	643.20	Joback Method
cpg	335.17	J/mol×K	609.25	Joback Method
cpg	322.49	J/mol×K	575.31	Joback Method
cpg	379.51	J/mol×K	745.03	Joback Method

dvisc	0.0004315	Pa×s	541.36	Joback Method
dvisc	0.0005049	Pa×s	506.87	Joback Method
dvisc	0.0006045	Pa×s	472.38	Joback Method
dvisc	0.0007447	Pa×s	437.89	Joback Method
dvisc	0.0009505	Pa×s	403.40	Joback Method
dvisc	0.0012700	Pa×s	368.91	Joback Method
dvisc	0.0018012	Pa×s	334.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3396201&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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