1,2-Cyclobutanedicarboxylic acid, dimethyl ester, cis-

Inchi: InChI=1S/C8H12O4/c1-11-7(9)5-3-4-6(5)8(10)12-2/h5-6H,3-4H2,1-2H3/t5-,6+
InchiKey: WEPHXFVXUXMCLE-OLQVQODUSA-N
Formula: C8H12O4
SMILES: COC(=O)C1CCC1C(=O)OC
Mol. weight [g/mol]: 172.18
CAS: 2607-03-6

Physical Properties

Property code	Value	Unit	Source
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	498.20	K	NIST Webbook
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	322.49	J/mol×K	575.31	Joback Method
cpg	335.17	J/mol×K	609.25	Joback Method
cpg	347.20	J/mol×K	643.20	Joback Method
cpg	358.61	J/mol×K	677.14	Joback Method
cpg	369.38	J/mol×K	711.09	Joback Method
cpg	379.51	J/mol×K	745.03	Joback Method
dvisc	0.0018012	Pa×s	334.42	Joback Method
dvisc	0.0012700	Pa×s	368.91	Joback Method

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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	387.20	K	2.70	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2607036&Units=SI

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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume