

Trans-1,2-cyclobutanedicarboxylic acid, dimethyl ester

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-/m1/s1
InchiKey:	WEPHXFVXUXMCLE-PHDIDXHHSA-N
Formula:	C8H12O4
SMILES:	COC(=O)C1CCC1C(=O)OC
Mol. weight [g/mol]:	172.18
CAS:	7371-67-7

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	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/molxK	541.36	Joback Method
cpg	322.49	J/molxK	575.31	Joback Method
cpg	335.17	J/molxK	609.25	Joback Method
cpg	347.20	J/molxK	643.20	Joback Method
cpg	358.61	J/molxK	677.14	Joback Method
cpg	369.38	J/molxK	711.09	Joback Method
cpg	379.51	J/molxK	745.03	Joback Method
dvisc	0.0018012	Paxs	334.42	Joback Method
dvisc	0.0012700	Paxs	368.91	Joback Method

dvisc	0.0009505	Paxs	403.40	Joback Method
dvisc	0.0007447	Paxs	437.89	Joback Method
dvisc	0.0006045	Paxs	472.38	Joback Method
dvisc	0.0005049	Paxs	506.87	Joback Method
dvisc	0.0004315	Paxs	541.36	Joback Method

Sources

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=C7371677&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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