Methylenedicarbamic acid, dimethyl ester

Inchi: InChI=1S/C5H10N2O4/c1-10-4(8)6-3-7-5(9)11-2/h3H2,1-2H3,(H,6,8)(H,7,9)
InchiKey: UPFCNJPMABXKFP-UHFFFAOYSA-N
Formula: C5H10N2O4
SMILES: COC(=O)NCNC(=O)OC
Mol. weight [g/mol]: 162.14
CAS: 5937-53-1

Physical Properties

Property code	Value	Unit	Source
gf	-297.84	kJ/mol	Joback Method
hf	-529.19	kJ/mol	Joback Method
hfus	24.48	kJ/mol	Joback Method
hvap	57.91	kJ/mol	Joback Method
log10ws	-0.47		Crippen Method
logp	-0.344		Crippen Method
mcvol	116.150	ml/mol	McGowan Method
pc	4005.77	kPa	Joback Method
tb	566.72	K	Joback Method
tc	760.06	K	Joback Method
tf	395.75	K	Joback Method
vc	0.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.76	J/mol×K	566.72	Joback Method
cpg	287.08	J/mol×K	598.94	Joback Method
cpg	296.00	J/mol×K	631.17	Joback Method
cpg	304.51	J/mol×K	663.39	Joback Method
cpg	312.60	J/mol×K	695.61	Joback Method
cpg	320.26	J/mol×K	727.84	Joback Method
cpg	327.47	J/mol×K	760.06	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5937531&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

Legend

cpg:	Ideal gas heat capacity
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