N,N-DIMETHYLGLYCINE METHYL ESTER

Other names: Methyl (dimethylamino) acetate
N,N-Dimethylglycine methyl ester
(CH3)2NCH2COOCH3
Inchi: InChI=1S/C5H11NO2/c1-6(2)4-5(7)8-3/h4H2,1-3H3
InchiKey: LRZFEBJUJIQVDQ-UHFFFAOYSA-N
Formula: C5H11NO2
SMILES: COC(=O)CN(C)C
Mol. weight [g/mol]: 117.15

Physical Properties

Property code	Value	Unit	Source
af	0.4009		Cheméo Relay (1.0)
chl	-3125.30 ± 0.63	kJ/mol	NIST Webbook
hf	-370.40 ± 0.79	kJ/mol	NIST Webbook
hfl	-414.30 ± 0.67	kJ/mol	NIST Webbook
hfus	14.51	kJ/mol	Joback Method
hvap	43.93 ± 0.46	kJ/mol	NIST Webbook
ie	7.96 ± 0.05	eV	NIST Webbook
ie	7.96 ± 0.03	eV	NIST Webbook
log10ws	0.73		Cheméo Relay (1.0)
logp	-0.279		Crippen Method
mcvol	98.730	ml/mol	McGowan Method
pc	3655.35	kPa	Joback Method
rinpol	809.00		NIST Webbook
rinpol	810.00		NIST Webbook
tb	388.56	K	Cheméo Relay (1.0)
tc	572.65	K	Cheméo Relay (1.0)
tf	197.86	K	Cheméo Relay (1.0)
vc	0.373	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	190.41	J/mol×K	402.53	Joback Method

cpg	200.15	J/mol×K	432.03	Joback Method
cpg	209.53	J/mol×K	461.53	Joback Method
cpg	218.57	J/mol×K	491.03	Joback Method
cpg	227.26	J/mol×K	520.53	Joback Method
cpg	235.61	J/mol×K	550.03	Joback Method
cpg	243.61	J/mol×K	579.52	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7148063&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor
chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume