L-Homoserine, N,O-dimethyl-, methyl ester

Other names: Methyl N,O-dimethyl-l-homoserinate
Inchi: InChI=1S/C7H15NO3/c1-8-6(4-5-10-2)7(9)11-3/h6,8H,4-5H2,1-3H3
InchiKey: FSGGHDZDWZFNKF-UHFFFAOYSA-N
Formula: C7H15NO3
SMILES: CNC(CCOC)C(=O)OC
Mol. weight [g/mol]: 161.20

Physical Properties

Property code	Value	Unit	Source
gf	-243.91	kJ/mol	Joback Method
hf	-516.64	kJ/mol	Joback Method
hfus	19.44	kJ/mol	Joback Method
hvap	48.79	kJ/mol	Joback Method
log10ws	-3.69e-03		Crippen Method
logp	-0.216		Crippen Method
mcvol	132.780	ml/mol	McGowan Method
pc	2953.69	kPa	Joback Method
rinpol	1418.80		NIST Webbook
rinpol	1418.80		NIST Webbook
tb	508.00	K	Joback Method
tc	690.56	K	Joback Method
tf	300.70	K	Joback Method
vc	0.498	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	306.87	J/mol×K	508.00	Joback Method
cpg	318.76	J/mol×K	538.43	Joback Method
cpg	330.22	J/mol×K	568.85	Joback Method
cpg	341.26	J/mol×K	599.28	Joback Method
cpg	351.87	J/mol×K	629.70	Joback Method
cpg	362.03	J/mol×K	660.13	Joback Method
cpg	371.76	J/mol×K	690.56	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=U332846&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume