Serine, methyl ester

Other names:	Methyl serinate
	Propanoic acid, 2-amino-3-hydroxy, methyl ester
Inchi:	InChI=1S/C4H9NO3/c1-8-4(7)3(5)2-6/h3,6H,2,5H2,1H3
InchiKey:	ANSUDRATXSJBLY-UHFFFAOYSA-N
Formula:	C4H9NO3
SMILES:	COC(=O)C(N)CO
Mol. weight [g/mol]:	119.12
CAS:	2104-89-4

Physical Properties

Property code	Value	Unit	Source
gf	-323.93	kJ/mol	Joback Method
hf	-494.41	kJ/mol	Joback Method
hfus	14.66	kJ/mol	Joback Method
hvap	60.59	kJ/mol	Joback Method
log10ws	0.83		Crippen Method
logp	-1.521		Crippen Method
mcvol	90.510	ml/mol	McGowan Method
pc	5109.34	kPa	Joback Method
rinpol	1034.00		NIST Webbook
rinpol	1032.00		NIST Webbook
rinpol	1038.00		NIST Webbook
rinpol	1034.00		NIST Webbook
tb	531.48	K	Joback Method
tc	719.71	K	Joback Method
tf	336.08	K	Joback Method
vc	0.326	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	210.91	J/mol×K	531.48	Joback Method
cpg	218.24	J/mol×K	562.85	Joback Method
cpg	225.26	J/mol×K	594.22	Joback Method

cpg	231.99	J/mol×K	625.60	Joback Method
cpg	238.41	J/mol×K	656.97	Joback Method
cpg	244.52	J/mol×K	688.34	Joback Method
cpg	250.33	J/mol×K	719.71	Joback Method

Sources

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=C2104894&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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