Glycine, n-(2-mercaptoethyl)-, methyl ester

Inchi: InChI=1S/C5H11NO2S/c1-8-5(7)4-6-2-3-9/h6,9H,2-4H2,1H3
InchiKey: RHPWTNYPTPZAGI-UHFFFAOYSA-N
Formula: C5H11NO2S
SMILES: COC(=O)CNCCS
Mol. weight [g/mol]: 149.21
CAS: 116435-39-3

Physical Properties

Property code	Value	Unit	Source
gf	-123.92	kJ/mol	Joback Method
hf	-299.38	kJ/mol	Joback Method
hfus	20.63	kJ/mol	Joback Method
hvap	49.05	kJ/mol	Joback Method
log10ws	-0.04		Crippen Method
logp	-0.321		Crippen Method
mcvol	115.080	ml/mol	McGowan Method
pc	4031.24	kPa	Joback Method
tb	503.12	K	Joback Method
tc	706.99	K	Joback Method
tf	307.39	K	Joback Method
vc	0.428	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	244.08	J/mol×K	503.12	Joback Method
cpg	254.08	J/mol×K	537.10	Joback Method
cpg	263.65	J/mol×K	571.08	Joback Method
cpg	272.79	J/mol×K	605.06	Joback Method
cpg	281.49	J/mol×K	639.03	Joback Method
cpg	289.75	J/mol×K	673.01	Joback Method
cpg	297.58	J/mol×K	706.99	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=C116435393&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume