N-Ethyl O-ethyl thiocarbamate

Inchi: InChI=1S/C5H11NOS/c1-3-6-5(8)7-4-2/h3-4H2,1-2H3,(H,6,8)
InchiKey: CMGLSTYFWSQNEC-UHFFFAOYSA-N
Formula: C5H11NOS
SMILES: CCNC(=S)OCC
Mol. weight [g/mol]: 133.21
CAS: 998-98-1

Physical Properties

Property code	Value	Unit	Source
gf	92.67	kJ/mol	Joback Method
hf	-78.78	kJ/mol	Joback Method
hfus	19.60	kJ/mol	Joback Method
hvap	42.30	kJ/mol	Joback Method
log10ws	-1.54		Crippen Method
logp	0.917		Crippen Method
mcvol	109.210	ml/mol	McGowan Method
pc	3857.88	kPa	Joback Method
rinpol	1121.00		NIST Webbook
ripol	1878.00		NIST Webbook
ripol	1878.00		NIST Webbook
tb	456.43	K	Joback Method
tc	655.16	K	Joback Method
tf	255.27	K	Joback Method
vc	0.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.31	J/mol×K	456.43	Joback Method
cpg	226.17	J/mol×K	489.55	Joback Method
cpg	235.51	J/mol×K	522.67	Joback Method
cpg	244.36	J/mol×K	555.79	Joback Method
cpg	252.75	J/mol×K	588.91	Joback Method
cpg	260.69	J/mol×K	622.03	Joback Method

cpg	268.21	J/mol×K	655.16	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=C998981&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume