N-Ethyl O-propyl thiocarbamate

Inchi: InChI=1S/C6H13NOS/c1-3-5-8-6(9)7-4-2/h3-5H2,1-2H3,(H,7,9)
InchiKey: SWDYQJANDQUWFH-UHFFFAOYSA-N
Formula: C6H13NOS
SMILES: CCCOC(=S)NCC
Mol. weight [g/mol]: 147.24

Physical Properties

Property code	Value	Unit	Source
gf	101.09	kJ/mol	Joback Method
hf	-99.42	kJ/mol	Joback Method
hfus	22.19	kJ/mol	Joback Method
hvap	44.53	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.307		Crippen Method
mcvol	123.300	ml/mol	McGowan Method
pc	3435.91	kPa	Joback Method
rinpol	1219.00		NIST Webbook
ripol	1970.00		NIST Webbook
tb	479.31	K	Joback Method
tc	675.64	K	Joback Method
tf	266.54	K	Joback Method
vc	0.461	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.61	J/mol×K	479.31	Joback Method
cpg	267.63	J/mol×K	512.03	Joback Method
cpg	278.09	J/mol×K	544.75	Joback Method
cpg	288.01	J/mol×K	577.47	Joback Method
cpg	297.41	J/mol×K	610.19	Joback Method
cpg	306.33	J/mol×K	642.92	Joback Method
cpg	314.78	J/mol×K	675.64	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R440038&Units=SI

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