N-Allyl O-propyl thiocarbamate

Inchi: InChI=1S/C7H13NOS/c1-3-5-8-7(10)9-6-4-2/h3H,1,4-6H2,2H3,(H,8,10)
InchiKey: BRQFNNQUZPSLIR-UHFFFAOYSA-N
Formula: C7H13NOS
SMILES: C=CCNC(=S)OCCC
Mol. weight [g/mol]: 159.25
CAS: 89895-26-1

Physical Properties

Property code	Value	Unit	Source
gf	197.35	kJ/mol	Joback Method
hf	5.37	kJ/mol	Joback Method
hfus	23.50	kJ/mol	Joback Method
hvap	46.08	kJ/mol	Joback Method
log10ws	-2.23		Crippen Method
logp	1.474		Crippen Method
mcvol	133.090	ml/mol	McGowan Method
pc	3228.31	kPa	Joback Method
rinpol	1286.00		NIST Webbook
ripol	2069.00		NIST Webbook
ripol	2069.00		NIST Webbook
tb	498.87	K	Joback Method
tc	696.81	K	Joback Method
tf	276.05	K	Joback Method
vc	0.497	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.17	J/mol×K	498.87	Joback Method
cpg	292.56	J/mol×K	531.86	Joback Method
cpg	303.31	J/mol×K	564.85	Joback Method
cpg	313.48	J/mol×K	597.84	Joback Method
cpg	323.08	J/mol×K	630.83	Joback Method
cpg	332.16	J/mol×K	663.82	Joback Method

cpg	340.75	J/mol×K	696.81	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=C89895261&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