Carbamodithioic acid, dimethyl, propyl ester

Inchi: InChI=1S/C6H13NS2/c1-4-5-9-6(8)7(2)3/h4-5H2,1-3H3
InchiKey: DAFYGLFCAJUUGS-UHFFFAOYSA-N
Formula: C6H13NS2
SMILES: CCCSC(=S)N(C)C
Mol. weight [g/mol]: 163.30

Physical Properties

Property code	Value	Unit	Source
gf	260.60	kJ/mol	Joback Method
hf	88.73	kJ/mol	Joback Method
hfus	23.05	kJ/mol	Joback Method
hvap	44.54	kJ/mol	Joback Method
log10ws	-2.13		Crippen Method
logp	1.976		Crippen Method
mcvol	133.780	ml/mol	McGowan Method
pc	3513.74	kPa	Joback Method
rinpol	1492.00		NIST Webbook
rinpol	1492.00		NIST Webbook
tb	487.94	K	Joback Method
tc	702.77	K	Joback Method
tf	258.52	K	Joback Method
vc	0.479	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	269.77	J/mol×K	487.94	Joback Method
cpg	282.01	J/mol×K	523.75	Joback Method
cpg	293.46	J/mol×K	559.55	Joback Method
cpg	304.16	J/mol×K	595.36	Joback Method
cpg	314.17	J/mol×K	631.16	Joback Method
cpg	323.53	J/mol×K	666.97	Joback Method
cpg	332.29	J/mol×K	702.77	Joback Method

Sources

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=R8601&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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