Propyl methylaminodithiocarbamate

Inchi: InChI=1S/C5H11NS2/c1-3-4-8-5(7)6-2/h3-4H2,1-2H3,(H,6,7)
InchiKey: KUDJTSQPXXVPAQ-UHFFFAOYSA-N
Formula: C5H11NS2
SMILES: CCCSC(=S)NC
Mol. weight [g/mol]: 149.28

Physical Properties

Property code	Value	Unit	Source
gf	230.79	kJ/mol	Joback Method
hf	95.31	kJ/mol	Joback Method
hfus	22.54	kJ/mol	Joback Method
hvap	46.71	kJ/mol	Joback Method
log10ws	-2.34		Crippen Method
logp	1.634		Crippen Method
mcvol	119.690	ml/mol	McGowan Method
pc	4026.13	kPa	Joback Method
rinpol	1507.00		NIST Webbook
rinpol	1516.00		NIST Webbook
rinpol	1521.00		NIST Webbook
rinpol	1518.00		NIST Webbook
rinpol	1507.00		NIST Webbook
rinpol	1509.00		NIST Webbook
rinpol	1512.00		NIST Webbook
rinpol	1521.00		NIST Webbook
tb	502.79	K	Joback Method
tc	725.26	K	Joback Method
tf	267.44	K	Joback Method
vc	0.441	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.58	J/mol×K	502.79	Joback Method
cpg	249.00	J/mol×K	539.87	Joback Method

cpg	258.76	J/mol×K	576.95	Joback Method
cpg	267.88	J/mol×K	614.03	Joback Method
cpg	276.41	J/mol×K	651.10	Joback Method
cpg	284.39	J/mol×K	688.18	Joback Method
cpg	291.87	J/mol×K	725.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R11228&Units=SI
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

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