Carbamodithioic acid, diethyl-, propyl ester

Other names: Carbamic acid, diethyldithio-, propyl ester
N,N-Diethyl S-propyl dithiocarbamate
S-Propyl N,N-diethyldithiocarbamate
Inchi: InChI=1S/C8H17NS2/c1-4-7-11-8(10)9(5-2)6-3/h4-7H2,1-3H3
InchiKey: YSSAGHQOEYPLQO-UHFFFAOYSA-N
Formula: C8H17NS2
SMILES: CCCSC(=S)N(CC)CC
Mol. weight [g/mol]: 191.36
CAS: 19047-77-9

Physical Properties

Property code	Value	Unit	Source
gf	277.44	kJ/mol	Joback Method
hf	47.45	kJ/mol	Joback Method
hfus	28.23	kJ/mol	Joback Method
hvap	48.99	kJ/mol	Joback Method
log10ws	-2.97		Crippen Method
logp	2.756		Crippen Method
mcvol	161.960	ml/mol	McGowan Method
pc	2832.35	kPa	Joback Method
rinpol	1569.00		NIST Webbook
rinpol	1520.00		NIST Webbook
tb	533.70	K	Joback Method
tc	741.93	K	Joback Method
tf	281.06	K	Joback Method
vc	0.592	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	357.48	J/mol×K	533.70	Joback Method
cpg	371.57	J/mol×K	568.41	Joback Method
cpg	384.80	J/mol×K	603.11	Joback Method
cpg	397.24	J/mol×K	637.82	Joback Method

cpg	408.92	J/mol×K	672.52	Joback Method
cpg	419.90	J/mol×K	707.23	Joback Method
cpg	430.23	J/mol×K	741.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19047779&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