

Carbamodithioic acid, dimethyl-, ethyl ester

Other names:	Carbamic acid, dimethyldithio-, ethyl ester Dimethyldithiocarbamic acid ethyl ester Ethyl dimethyldithiocarbamate Preparation 23 Ethyl ester of dimethyldithiocarbamic acid S-Ethyl-N,N-dimethyldithiocarbamate
Inchi:	InChI=1S/C5H11NS2/c1-4-8-5(7)6(2)3/h4H2,1-3H3
InchiKey:	VPNCITAAFVUKG-UHFFFAOYSA-N
Formula:	C5H11NS2
SMILES:	CCSC(=S)N(C)C
Mol. weight [g/mol]:	149.28
CAS:	617-38-9

Physical Properties

Property code	Value	Unit	Source
chl	-4694.40	kJ/mol	NIST Webbook
gf	252.18	kJ/mol	Joback Method
hf	109.37	kJ/mol	Joback Method
hfl	-46.90	kJ/mol	NIST Webbook
hfus	20.46	kJ/mol	Joback Method
hvap	42.31	kJ/mol	Joback Method
log10ws	-1.72		Crippen Method
logp	1.586		Crippen Method
mcvol	119.690	ml/mol	McGowan Method
pc	3950.57	kPa	Joback Method
tb	465.06	K	Joback Method
tc	683.19	K	Joback Method
tf	247.25	K	Joback Method
vc	0.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.81	J/molxK	465.06	Joback Method

cpg	239.92	J/mol×K	501.41	Joback Method
cpg	250.29	J/mol×K	537.77	Joback Method
cpg	259.95	J/mol×K	574.12	Joback Method
cpg	268.95	J/mol×K	610.48	Joback Method
cpg	277.34	J/mol×K	646.83	Joback Method
cpg	285.17	J/mol×K	683.19	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C617389&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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