

Carbamodithioic acid, diethyl-

Other names:	Carbamic acid, diethyldithio- Dieca Diethyldithiocarbamic acid Diethyldithiocarbaminic acid Diethyldithione
Inchi:	InChI=1S/C5H11NS2/c1-3-6(4-2)5(7)8/h3-4H2,1-2H3,(H,7,8)
InchiKey:	LMBWSYZSUOEYSN-UHFFFAOYSA-N
Formula:	C5H11NS2
SMILES:	CCN(CC)C(=S)S
Mol. weight [g/mol]:	149.28
CAS:	147-84-2

Physical Properties

Property code	Value	Unit	Source
gf	248.45	kJ/mol	Joback Method
hf	33.20 ± 3.80	kJ/mol	NIST Webbook
hfus	20.37	kJ/mol	Joback Method
hvap	42.23	kJ/mol	Joback Method
log10ws	-1.90		Crippen Method
logp	1.543		Crippen Method
mcpvol	119.690	ml/mol	McGowan Method
pc	4194.74	kPa	Joback Method
tb	459.14	K	Joback Method
tc	677.45	K	Joback Method
tf	249.31	K	Joback Method
vc	0.423	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.33	J/mol×K	459.14	Joback Method
cpg	238.43	J/mol×K	495.52	Joback Method
cpg	248.74	J/mol×K	531.91	Joback Method
cpg	258.30	J/mol×K	568.29	Joback Method

cpg	267.18	J/mol×K	604.68	Joback Method
cpg	275.44	J/mol×K	641.06	Joback Method
cpg	283.14	J/mol×K	677.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C147842&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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