

Carbamodithioic acid, diethyl-, ethyl ester

Other names:	Carbamic acid, diethyldithio-, ethyl ester Diethyldithiocarbamic acid ethyl ester S-Ethyl-N,N-diethyldithiocarbamate
Inchi:	InChI=1S/C7H15NS2/c1-4-8(5-2)7(9)10-6-3/h4-6H2,1-3H3
InchiKey:	RKDROQWWHWDICV-UHFFFAOYSA-N
Formula:	C7H15NS2
SMILES:	CCSC(=S)N(CC)CC
Mol. weight [g/mol]:	177.33
CAS:	4740-11-8

Physical Properties

Property code	Value	Unit	Source
gf	269.02	kJ/mol	Joback Method
hf	68.09	kJ/mol	Joback Method
hfus	25.64	kJ/mol	Joback Method
hvap	46.77	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	2.366		Crippen Method
mcvol	147.870	ml/mol	McGowan Method
pc	3145.56	kPa	Joback Method
tb	510.82	K	Joback Method
tc	722.33	K	Joback Method
tf	269.79	K	Joback Method
vc	0.535	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.70	J/molxK	510.82	Joback Method
cpg	325.92	J/molxK	546.07	Joback Method
cpg	338.32	J/molxK	581.32	Joback Method
cpg	349.95	J/molxK	616.58	Joback Method
cpg	360.84	J/molxK	651.83	Joback Method
cpg	371.06	J/molxK	687.08	Joback Method

Sources

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=C4740118&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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