

Ethane, 1,1'-[methylenebis(thio)]bis-

Other names:	1,1-bis(Ethylthio)methane 3,5-Dithiaheptane Bis(ethylthio)methane <chem>C2H5SCH2SC2H5</chem> Di(ethylthio)methane Formaldehyde diethyl mercaptal Methane, bis(ethylthio)-
Inchi:	InChI=1S/C5H12S2/c1-3-6-5-7-4-2/h3-5H2,1-2H3
InchiKey:	RJQVVQDWHKZIHU-UHFFFAOYSA-N
Formula:	C5H12S2
SMILES:	CCSCSCC
Mol. weight [g/mol]:	136.28
CAS:	4396-19-4

Physical Properties

Property code	Value	Unit	Source
chl	-4770.50 ± 1.10	kJ/mol	NIST Webbook
gf	57.46	kJ/mol	Joback Method
hf	-65.20 ± 1.50	kJ/mol	NIST Webbook
hfl	-116.00 ± 1.50	kJ/mol	NIST Webbook
hfus	16.97	kJ/mol	Joback Method
hvap	50.80	kJ/mol	NIST Webbook
hvap	50.80 ± 0.16	kJ/mol	NIST Webbook
hvap	50.80	kJ/mol	NIST Webbook
ie	8.22 ± 0.02	eV	NIST Webbook
ie	8.66	eV	NIST Webbook
log10ws	-2.18		Crippen Method
logp	2.450		Crippen Method
mcvol	114.010	ml/mol	McGowan Method
pc	3611.55	kPa	Joback Method
rinpol	1054.00		NIST Webbook
rinpol	1055.00		NIST Webbook
tb	451.36	K	Joback Method
tc	666.63	K	Joback Method
tf	214.91	K	Joback Method
vc	0.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.79	J/mol×K	451.36	Joback Method
cpg	224.75	J/mol×K	487.24	Joback Method
cpg	235.26	J/mol×K	523.12	Joback Method
cpg	245.30	J/mol×K	558.99	Joback Method
cpg	254.88	J/mol×K	594.87	Joback Method
cpg	264.00	J/mol×K	630.75	Joback Method
cpg	272.66	J/mol×K	666.63	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.45427e+01
Coeff. B	-3.76564e+03
Coeff. C	-6.43390e+01
Temperature range (K), min.	328.50
Temperature range (K), max.	472.26

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=C4396194&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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