Ethane, 1,2-bis(methylthio)-

Other names:	1,2-Bis(methylmercapto)ethane
	1,2-Bis(methylthio)ethane
	2,5-Dithiahexane
	CH3SCH2CH2SCH3
Inchi:	InChI=1S/C4H10S2/c1-5-3-4-6-2/h3-4H2,1-2H3
InchiKey:	UJTDKNZVLGVLFT-UHFFFAOYSA-N
Formula:	C4H10S2
SMILES:	CSCCSC
Mol. weight [g/mol]:	122.25
CAS:	6628-18-8

Physical Properties

Property code	Value	Unit	Source
gf	49.04	kJ/mol	Joback Method
hf	-42.15	kJ/mol	Joback Method
hfus	14.38	kJ/mol	Joback Method
hvap	38.13	kJ/mol	Joback Method
log10ws	-1.26		Crippen Method
logp	1.712		Crippen Method
mcvol	99.920	ml/mol	McGowan Method
pc	4067.32	kPa	Joback Method
rinpol	1027.00		NIST Webbook
rinpol	1029.00		NIST Webbook
ripol	1479.00		NIST Webbook
tb	428.48	K	Joback Method
tc	646.67	K	Joback Method
tf	203.64	K	Joback Method
vc	0.367	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	175.81	J/mol×K	428.48	Joback Method
cpg	185.27	J/mol×K	464.85	Joback Method

cpg	194.36	J/mol×K	501.21	Joback Method
cpg	203.07	J/mol×K	537.58	Joback Method
cpg	211.40	J/mol×K	573.94	Joback Method
cpg	219.35	J/mol×K	610.31	Joback Method
cpg	226.91	J/mol×K	646.67	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.81852e+01
Coeff. B	-4.79193e+03
Coeff. C	-6.76820e+01
Temperature range (K), min.	335.42
Temperature range (K), max.	439.91

Sources

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=C6628188&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/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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