

Bis(chloromethyl) sulfide

Inchi:	InChI=1S/C2H4Cl2S/c3-1-5-2-4/h1-2H2
InchiKey:	KRIFIIWBVJKVST-UHFFFAOYSA-N
Formula:	C2H4Cl2S
SMILES:	CICSCCI
Mol. weight [g/mol]:	131.02
CAS:	3592-44-7

Physical Properties

Property code	Value	Unit	Source
gf	-24.78	kJ/mol	Joback Method
hf	-74.22	kJ/mol	Joback Method
hfus	13.46	kJ/mol	Joback Method
hvap	35.63	kJ/mol	Joback Method
log10ws	-1.84		Crippen Method
logp	2.112		Crippen Method
mcvol	79.870	ml/mol	McGowan Method
pc	4646.65	kPa	Joback Method
tb	388.80	K	Joback Method
tc	600.72	K	Joback Method
tf	206.54	K	Joback Method
vc	0.299	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	133.72	J/mol×K	565.40	Joback Method
cpg	112.14	J/mol×K	388.80	Joback Method
cpg	116.87	J/mol×K	424.12	Joback Method
cpg	121.38	J/mol×K	459.44	Joback Method
cpg	125.70	J/mol×K	494.76	Joback Method
cpg	129.81	J/mol×K	530.08	Joback Method
cpg	137.43	J/mol×K	600.72	Joback Method
hvapt	45.10	kJ/mol	375.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.73866e+01
Coeff. B	-5.48811e+03
Temperature range (K), min.	320.00
Temperature range (K), max.	454.50

Sources

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
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=C3592447&Units=SI

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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