

Propane, 1-chloro-3-((2-chloroethyl)thio)-

Other names:	1-Chloro-3-((2-chloroethyl)thio)propane 2-Chloroethyl-3-chloropropyl sulfide
Inchi:	InChI=1S/C5H10Cl2S/c6-2-1-4-8-5-3-7/h1-5H2
InchiKey:	NXRPRUPNFDEDSY-UHFFFAOYSA-N
Formula:	C5H10Cl2S
SMILES:	C1CCCSCCCI
Mol. weight [g/mol]:	173.10
CAS:	71784-01-5

Physical Properties

Property code	Value	Unit	Source
gf	0.48	kJ/mol	Joback Method
hf	-136.14	kJ/mol	Joback Method
hfus	21.23	kJ/mol	Joback Method
hvap	42.31	kJ/mol	Joback Method
log10ws	-2.11		Crippen Method
logp	2.587		Crippen Method
mcpvol	122.140	ml/mol	McGowan Method
pc	3246.73	kPa	Joback Method
rinpol	1169.00		NIST Webbook
rinpol	1212.60		NIST Webbook
rinpol	1174.00		NIST Webbook
rinpol	1169.00		NIST Webbook
rinpol	1212.60		NIST Webbook
tb	457.44	K	Joback Method
tc	662.27	K	Joback Method
tf	240.35	K	Joback Method
vc	0.468	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.04	J/molxK	457.44	Joback Method
cpg	227.50	J/molxK	491.58	Joback Method

cpg	236.50	J/mol×K	525.72	Joback Method
cpg	245.07	J/mol×K	559.86	Joback Method
cpg	253.20	J/mol×K	594.00	Joback Method
cpg	260.92	J/mol×K	628.14	Joback Method
cpg	268.23	J/mol×K	662.27	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C71784015&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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	McGowan's characteristic volume
pc:	Critical Pressure
r inpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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