Propane, 1-chloro-3-(2-chloroethylthio)-

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: ClCCCSCCCl
Mol. weight [g/mol]: 173.11

Physical Properties

Property code	Value	Unit	Source
af	0.3935		Cheméo Relay (1.0)
hf	-151.32	kJ/mol	Cheméo Relay (1.0)
hfus	21.23	kJ/mol	Joback Method
hvap	62.00	kJ/mol	Cheméo Relay (1.0)
ie	9.33	eV	Cheméo Relay (1.0)
log10ws	-2.39		Cheméo Relay (1.0)
logp	2.587		Crippen Method
mcvol	122.140	ml/mol	McGowan Method
pc	3246.73	kPa	Joback Method
rinpol	1212.60		NIST Webbook
rinpol	1169.00		NIST Webbook
rinpol	1169.00		NIST Webbook
rinpol	1212.60		NIST Webbook
rinpol	1174.00		NIST Webbook
tb	497.49	K	Cheméo Relay (1.0)
tc	716.52	K	Cheméo Relay (1.0)
tf	226.97	K	Cheméo Relay (1.0)
vc	0.428	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C71784015&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
hf: 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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume