Trisulfide, bis(2-chloroethyl)-

Other names:	Trisulfane, 1,3-di(2-chloroethyl)-
	1,3-Bis(2-chloroethyl)trisulfane
	bis-(2-Chloroethyl) trisulfide
Inchi:	InChI=1S/C4H8Cl2S3/c5-1-3-7-9-8-4-2-6/h1-4H2
InchiKey:	XHODIRQQNWHUGV-UHFFFAOYSA-N
Formula:	C4H8Cl2S3
SMILES:	ClCCSSSCCCl
Mol. weight [g/mol]:	223.21
CAS:	19149-77-0

Physical Properties

Property code	Value	Unit	Source
gf	58.30	kJ/mol	Joback Method
hf	-31.76	kJ/mol	Joback Method
hfus	26.90	kJ/mol	Joback Method
hvap	53.72	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	3.494		Crippen Method
mcvol	140.750	ml/mol	McGowan Method
pc	3786.98	kPa	Joback Method
rinpol	1562.00		NIST Webbook
rinpol	1626.30		NIST Webbook
rinpol	1626.30		NIST Webbook
rinpol	1561.70		NIST Webbook
rinpol	1562.00		NIST Webbook
rinpol	1626.30		NIST Webbook
rinpol	1562.00		NIST Webbook
rinpol	1626.30		NIST Webbook
ripol	2456.20		NIST Webbook
ripol	2456.20		NIST Webbook
tb	572.12	K	Joback Method
tc	824.18	K	Joback Method
tf	297.88	K	Joback Method
vc	0.519	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.93	J/mol×K	572.12	Joback Method
cpg	267.98	J/mol×K	614.13	Joback Method
cpg	276.44	J/mol×K	656.14	Joback Method
cpg	284.30	J/mol×K	698.15	Joback Method
cpg	291.55	J/mol×K	740.16	Joback Method
cpg	298.17	J/mol×K	782.17	Joback Method
cpg	304.16	J/mol×K	824.18	Joback Method
hvapt	68.20	kJ/mol	313.00	NIST Webbook

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=C19149770&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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