Tris(2-chloroethyl)amine

Other names:	HN3
	Trichlormethine
	A 8729
	Ethanamine, 2-chloro-N,N-bis(2-chloroethyl)-
	Sinalost base
	SK 100
	Tri-2-chloroethylamine
	Triethylamine, 2,2',2''-trichloro-
	Trimitan base
	Tris(«beta»-chloroethyl)amine
	TL 145
	TS 160
	2,2',2''-Trichlorotriethylamine
	Trimustine
	Lekamin
	NSC-260424
	bis(2-chloroethyl)acetaldehyde acetal
Inchi:	InChI=1S/C6H12Cl3N/c7-1-4-10(5-2-8)6-3-9/h1-6H2
InchiKey:	FDAYLTPAFBGXAB-UHFFFAOYSA-N
Formula:	C6H12Cl3N
SMILES:	ClCCN(CCCl)CCCl
Mol. weight [g/mol]:	204.53
CAS:	555-77-1

Physical Properties

Property code	Value	Unit	Source
gf	74.63	kJ/mol	Joback Method
hf	-146.86	kJ/mol	Joback Method
hfus	26.91	kJ/mol	Joback Method
hvap	44.15	kJ/mol	Joback Method
log10ws	-1.36		Crippen Method
logp	2.005		Crippen Method
mcvol	142.100	ml/mol	McGowan Method
pc	2749.78	kPa	Joback Method
rinpol	1411.00		NIST Webbook
rinpol	1405.00		NIST Webbook
rinpol	1361.00		NIST Webbook

rinpol	1405.37		NIST Webbook
rinpol	1403.83		NIST Webbook
rinpol	1411.00		NIST Webbook
rinpol	1361.00		NIST Webbook
rinpol	1405.00		NIST Webbook
ripol	2101.00		NIST Webbook
ripol	2070.40		NIST Webbook
ripol	2089.00		NIST Webbook
tb	461.41	K	Joback Method
tc	646.27	K	Joback Method
tf	279.61	K	Joback Method
vc	0.536	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.97	J/mol×K	615.46	Joback Method
cpg	267.57	J/mol×K	461.41	Joback Method
cpg	278.32	J/mol×K	492.22	Joback Method
cpg	288.51	J/mol×K	523.03	Joback Method
cpg	298.17	J/mol×K	553.84	Joback Method
cpg	307.31	J/mol×K	584.65	Joback Method
cpg	324.16	J/mol×K	646.27	Joback Method
hvapt	65.00	kJ/mol	303.00	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=C555771&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