Ethyl-bis(2-chloroethyl)amine

Other names:	2,2'-Dichlorotriethylamine Ethanamine, 2-chloro-N-(2-chloroethyl)-N-ethyl- Ethyl-S Ethylbis(2-chloroethyl)amine Ethylbis(«beta»-chloroethyl)amine HN1 Nitrogen mustard (HN-1) TL 1149 TL 329 Triethylamine, 2,2'-dichloro- bis(2-chloroethyl)ethylamine
Inchi:	InChI=1S/C6H13Cl2N/c1-2-9(5-3-7)6-4-8/h2-6H2,1H3
InchiKey:	UQZPGHOJMQTOHB-UHFFFAOYSA-N
Formula:	C6H13Cl2N
SMILES:	CCN(CCCl)CCCl
Mol. weight [g/mol]:	170.08
CAS:	538-07-8

Physical Properties

Property code	Value	Unit	Source
af	0.4284		Cheméo Relay (1.0)
gf	86.56	kJ/mol	Joback Method
hf	-143.53	kJ/mol	Cheméo Relay (1.0)
hfus	22.71	kJ/mol	Joback Method
hvap	50.30	kJ/mol	Cheméo Relay (1.0)
ie	8.60	eV	Cheméo Relay (1.0)
log10ws	-1.41		Cheméo Relay (1.0)
logp	1.786		Crippen Method
mcvol	129.860	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
rinpol	1156.00		NIST Webbook
rinpol	1153.33		NIST Webbook
rinpol	1152.50		NIST Webbook
rinpol	1156.00		NIST Webbook
rinpol	1156.00		NIST Webbook
tb	461.38	K	Cheméo Relay (1.0)
tc	645.81	K	Cheméo Relay (1.0)

tf	206.07	K	Cheméo Relay (1.0)
vc	0.450	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	240.95	J/mol×K	423.98	Joback Method
cpg	252.18	J/mol×K	453.70	Joback Method
cpg	262.89	J/mol×K	483.43	Joback Method
cpg	273.08	J/mol×K	513.15	Joback Method
cpg	282.79	J/mol×K	542.87	Joback Method
cpg	292.02	J/mol×K	572.60	Joback Method
cpg	300.80	J/mol×K	602.32	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.25244e+01
Coeff. B	-4.37791e+03
Temperature range (K), min.	357.77
Temperature range (K), max.	606.96

Sources

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C538078&Units=SI

Legend

af:	Acentric Factor
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume