chlornaphazine

Inchi: InChI=1S/C14H15Cl2N/c15-7-9-17(10-8-16)14-6-5-12-3-1-2-4-13(12)11-14/h1-6,11H,7-1
InchiKey: XCDXSSFOJZZGQC-UHFFFAOYSA-N
Formula: C14H15Cl2N
SMILES: ClCCN(CCCl)c1ccc2ccccc2c1
Mol. weight [g/mol]: 268.18
CAS: 494-03-1

Physical Properties

Property code	Value	Unit	Source
gf	363.35	kJ/mol	Joback Method
hf	119.89	kJ/mol	Joback Method
hfus	34.10	kJ/mol	Joback Method
hvap	62.15	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	4.124		Crippen Method
mcvol	199.360	ml/mol	McGowan Method
pc	2318.07	kPa	Joback Method
tb	657.66	K	Joback Method
tc	883.23	K	Joback Method
tf	328.00 ± 1.00	K	NIST Webbook
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	482.48	J/mol×K	657.66	Joback Method
cpg	497.09	J/mol×K	695.26	Joback Method
cpg	510.62	J/mol×K	732.85	Joback Method
cpg	523.16	J/mol×K	770.45	Joback Method
cpg	534.81	J/mol×K	808.04	Joback Method
cpg	545.67	J/mol×K	845.64	Joback Method
cpg	555.81	J/mol×K	883.23	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	483.20	K	0.70	NIST Webbook
tbrp	483.00	K	0.70	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C494031&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume