

Morpholine, 4-(2-chloroethyl)-

Other names:	4-(2-Chloroethyl)morpholine N-(2-Chloroethyl)morpholine TL 401
Inchi:	InChI=1S/C6H12ClNO/c7-1-2-8-3-5-9-6-4-8/h1-6H2
InchiKey:	ZAPMTSHEXFEPSP-UHFFFAOYSA-N
Formula:	C6H12ClNO
SMILES:	CICCN1CCOCC1
Mol. weight [g/mol]:	149.62
CAS:	3240-94-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.04		Crippen Method
logp	0.557		Crippen Method
mcvol	112.630	ml/mol	McGowan Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.85234e+01
Coeff. B	-6.46727e+03
Temperature range (K), min.	354.65
Temperature range (K), max.	489.50

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3240946&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure

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<https://www.chemeo.com/cid/98-489-2/Morpholine-4-2-chloroethyl.pdf>

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