

Benzenamine, 2,6-dichloro-

Other names:	2,6-Dichloroaniline
Inchi:	InChI=1S/C6H5Cl2N/c7-4-2-1-3-5(8)6(4)9/h1-3H,9H2
InchiKey:	JDMFXJULNGEPOI-UHFFFAOYSA-N
Formula:	C6H5Cl2N
SMILES:	Nc1c(Cl)cccc1Cl
Mol. weight [g/mol]:	162.02
CAS:	608-31-1

Physical Properties

Property code	Value	Unit	Source
gf	135.38	kJ/mol	Joback Method
hf	48.73	kJ/mol	Joback Method
hfus	18.15	kJ/mol	Joback Method
hsub	74.20 ± 0.90	kJ/mol	NIST Webbook
hvap	51.96	kJ/mol	Joback Method
ie	7.60 ± 0.02	eV	NIST Webbook
log10ws	-2.48		Crippen Method
logp	2.576		Crippen Method
mcvol	106.100	ml/mol	McGowan Method
pc	4385.77	kPa	Joback Method
rinpol	1210.00		NIST Webbook
rinpol	1204.00		NIST Webbook
rinpol	1202.00		NIST Webbook
rinpol	1202.00		NIST Webbook
rinpol	1202.00		NIST Webbook
rinpol	1203.00		NIST Webbook
rinpol	1204.00		NIST Webbook
rinpol	1204.00		NIST Webbook
ripol	1905.00		NIST Webbook
ripol	1905.00		NIST Webbook
ripol	1905.00		NIST Webbook
tb	520.71	K	Joback Method
tc	765.61	K	Joback Method
tf	351.94	K	Joback Method
vc	0.391	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	191.63	J/mol×K	520.71	Joback Method
cpg	199.84	J/mol×K	561.53	Joback Method
cpg	207.47	J/mol×K	602.34	Joback Method
cpg	214.54	J/mol×K	643.16	Joback Method
cpg	221.09	J/mol×K	683.97	Joback Method
cpg	227.13	J/mol×K	724.79	Joback Method
cpg	232.70	J/mol×K	765.61	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C608311&Units=SI

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
hsub:	Enthalpy of sublimation 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
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

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