

Ethene, 1-bromo-1-chloro-

Inchi:	InChI=1S/C2H2BrCl/c1-2(3)4/h1H2
InchiKey:	DQIRHMDFDOXWHX-UHFFFAOYSA-N
Formula:	C2H2BrCl
SMILES:	C=C(Cl)Br
Mol. weight [g/mol]:	141.39
CAS:	17759-85-2

Physical Properties

Property code	Value	Unit	Source
gf	47.64	kJ/mol	Joback Method
hf	41.62	kJ/mol	Joback Method
hfus	7.83	kJ/mol	Joback Method
hvap	30.28	kJ/mol	Joback Method
log10ws	-2.09		Crippen Method
logp	2.091		Crippen Method
mcvol	64.480	ml/mol	McGowan Method
pc	5644.74	kPa	Joback Method
tb	345.31	K	Joback Method
tc	550.76	K	Joback Method
tf	186.30	K	Joback Method
vc	0.240	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	73.99	J/molxK	345.31	Joback Method
cpg	77.47	J/molxK	379.55	Joback Method
cpg	80.69	J/molxK	413.79	Joback Method
cpg	83.64	J/molxK	448.03	Joback Method
cpg	86.36	J/molxK	482.28	Joback Method
cpg	88.86	J/molxK	516.52	Joback Method
cpg	91.16	J/molxK	550.76	Joback Method

Sources

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=C17759852&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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