

Propanenitrile, 3-(trichlorosilyl)-

Other names:	2-Cyanoethyltrichlorosilane 3-(Trichlorosilyl)propanenitrile 3-(trichlorosilyl)propionitrile 3-Trichlorosilylpropionitrile Propionitrile, 3-(trichlorosilyl)- Silane, (2-cyanoethyl)trichloro- Trichlor-2-kyanethylsilan Trichloro(2-cyanoethyl)silane «beta»-Cyanoethyltrichlorosilane «beta»-Trichlorosilylpropionitrile Â«betaÂ»-Cyanoethyltrichlorosilane Â«betaÂ»-Trichlorosilylpropionitrile
Inchi:	InChI=1S/C3H4Cl3NSi/c4-8(5,6)3-1-2-7/h1,3H2
InchiKey:	OLBGECWYBGXCNV-UHFFFAOYSA-N
Formula:	C3H4Cl3NSi
SMILES:	N#CCC[Si](Cl)(Cl)Cl
Mol. weight [g/mol]:	188.51
CAS:	1071-22-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.62		Crippen Method
logp	2.555		Crippen Method
ss	246.00	J/mol×K	NIST Webbook
tt	307.90 ± 0.02	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	186.10	J/mol×K	298.15	NIST Webbook
hfust	21.24	kJ/mol	307.90	NIST Webbook
hfust	21.24	kJ/mol	307.90	NIST Webbook
sfust	69.00	J/mol×K	307.90	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	382.00	K	4.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.21853e+01
Coeff. B	-2.70031e+03
Coeff. C	-1.33610e+02
Temperature range (K), min.	342.00
Temperature range (K), max.	526.45

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1071223&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

cps:	Solid phase heat capacity
hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
pvap:	Vapor pressure
sfust:	Entropy of fusion at a given temperature

ss: Solid phase molar entropy at standard conditions
tbrp: Boiling point at reduced pressure
tt: Triple Point Temperature

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