

Trimethylsilyl fluoride

Other names:	(CH3)3SiF Fluorotrimethylsilane Silane, fluorotrimethyl- Trimethylfluorosilane Trimethylsilicon fluoride
Inchi:	InChI=1S/C3H9FSi/c1-5(2,3)4/h1-3H3
InchiKey:	CTIKAHQFRQTTAY-UHFFFAOYSA-N
Formula:	C3H9FSi
SMILES:	C[Si](C)(C)F
Mol. weight [g/mol]:	92.19
CAS:	420-56-4

Physical Properties

Property code	Value	Unit	Source
ie	11.00	eV	NIST Webbook
ie	10.31 ± 0.04	eV	NIST Webbook
ie	10.55 ± 0.06	eV	NIST Webbook
log10ws	1.02		Crippen Method
logp	1.791		Crippen Method
rinpol	437.00		NIST Webbook
rinpol	416.00		NIST Webbook
rinpol	416.00		NIST Webbook
tb	290.00 ± 1.00	K	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.57740e+01
Coeff. B	-3.23513e+03
Temperature range (K), min.	208.90
Temperature range (K), max.	309.21

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C420564&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/ci990307I
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

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