

4-Chloro-1-trimethylsilyloxybenzene

Other names:	4-Chloro-1-trimethylsilyloxybenzene 4-Chlorophenol, trimethylsilyl ether Phenol, 4-chloro, TMS
Inchi:	InChI=1S/C9H13ClOSi/c1-12(2,3)11-9-6-4-8(10)5-7-9/h4-7H,1-3H3
InchiKey:	CJDREQROIGYMMO-UHFFFAOYSA-N
Formula:	C9H13ClOSi
SMILES:	C[Si](C)(C)Oc1ccc(Cl)cc1
Mol. weight [g/mol]:	200.74

Physical Properties

Property code	Value	Unit	Source
hf	-294.98	kJ/mol	Cheméo Relay (1.0)
hvap	55.50	kJ/mol	Cheméo Relay (1.0)
ie	8.74	eV	Cheméo Relay (1.0)
log10ws	-3.21		Cheméo Relay (1.0)
logp	3.554		Crippen Method
rinpol	1244.00		NIST Webbook
rinpol	1218.00		NIST Webbook
rinpol	1245.70		NIST Webbook
rinpol	1220.00		NIST Webbook
tb	497.10	K	Cheméo Relay (1.0)
tf	289.67	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C17005593&Units=SI>

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

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

Cheméo Relay (1.0):

Legend

hf:	Enthalpy of formation at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log₁₀ws:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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