ETHYL (TRIMETHYLSILYL)ACETATE

Other names: Ethyl (2-trimethylsilyl)acetate
Acetic acid, (trimethylsilyl)-, ethyl ester
Inchi: InChI=1S/C7H16O2Si/c1-5-9-7(8)6-10(2,3)4/h5-6H2,1-4H3
InchiKey: QQFBQBDINHJDMN-UHFFFAOYSA-N
Formula: C7H16O2Si
SMILES: CCOC(=O)C[Si](C)(C)C
Mol. weight [g/mol]: 160.29

Physical Properties

Property code	Value	Unit	Source
af	0.4260		Cheméo Relay (1.0)
gf	-270.76	kJ/mol	Cheméo Relay (1.0, beta)
hf	-631.39	kJ/mol	Cheméo Relay (1.0)
hvap	46.86	kJ/mol	Cheméo Relay (1.0)
ie	9.33	eV	Cheméo Relay (1.0)
log10ws	-1.48		Cheméo Relay (1.0)
logp	1.888		Crippen Method
pc	2102.05	kPa	Cheméo Relay (1.0, beta)
rinpol	942.00		NIST Webbook
rinpol	930.00		NIST Webbook
tb	430.00 ± 1.00	K	NIST Webbook
tc	593.91	K	Cheméo Relay (1.0)
tf	225.55	K	Cheméo Relay (1.0)
vc	0.524	m3/kmol	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4071889&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation 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
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume