Glutaric acid, trimethylsilyl ester

Other names:	Glutaric acid, trimethylsilyl ester
	Monomethyl glutarate, tms derivative
Inchi:	InChI=1S/C9H18O4Si/c1-12-8(10)6-5-7-9(11)13-14(2,3)4/h5-7H2,1-4H3
InchiKey:	PPDBCMNNWDFEBX-UHFFFAOYSA-N
Formula:	C9H18O4Si
SMILES:	COC(=O)CCCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	218.33

Physical Properties

Property code	Value	Unit	Source
af	0.6026		Cheméo Relay (1.0)
hf	-959.85	kJ/mol	Cheméo Relay (1.0)
hvap	62.89	kJ/mol	Cheméo Relay (1.0)
ie	9.99	eV	Cheméo Relay (1.0)
log10ws	-1.22		Cheméo Relay (1.0)
logp	1.708		Crippen Method
pc	1697.03	kPa	Cheméo Relay (1.0, beta)
rinpol	1286.20		NIST Webbook
rinpol	1286.20		NIST Webbook
tb	496.51	K	Cheméo Relay (1.0)
tc	650.15	K	Cheméo Relay (1.0)
tf	250.89	K	Cheméo Relay (1.0)
vc	0.680	m3/kmol	Cheméo Relay (1.0)

Sources

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333977&Units=SI

Legend

af:	Acentric Factor
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