Acetic acid, isothiocyanato-, ethyl ester

Other names:	Carbethoxymethyl isothiocyanate
	Carboethoxymethyl isothiocyanate
	Ethyl isothiocyanatoacetate
	Ethyl isothiocyanoacetate
	Isothiocyanato-acetic acid ethyl ester
	Acetic acid, 2-isothiocyanato-, ethyl ester
	etil-izotiocianáto-acetát
Inchi:	InChI=1S/C5H7NO2S/c1-2-8-5(7)3-6-4-9/h2-3H2,1H3
InchiKey:	IYPSSPPKMLXXRN-UHFFFAOYSA-N
Formula:	C5H7NO2S
SMILES:	CCOC(=O)CN=C=S
Mol. weight [g/mol]:	145.18
CAS:	24066-82-8

Physical Properties

Property code	Value	Unit	Source
hf	-107.26	kJ/mol	Joback Method
hvap	46.32	kJ/mol	Joback Method
log10ws	-0.71		Crippen Method
logp	0.652		Crippen Method
mcvol	106.480	ml/mol	McGowan Method
pc	3763.78	kPa	Joback Method
rinpol	1149.30		NIST Webbook
rinpol	1149.30		NIST Webbook
tb	536.04	K	Joback Method
tc	761.37	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24066828&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature