Ethyl 2-isothiocyanatoacetate

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

Physical Properties

Property code	Value	Unit	Source
af	0.4014		Cheméo Relay (1.0)
gf	-97.48	kJ/mol	Cheméo Relay (1.0, beta)
hf	-198.74	kJ/mol	Cheméo Relay (1.0)
hvap	59.96	kJ/mol	Cheméo Relay (1.0)
ie	8.98	eV	Cheméo Relay (1.0)
log10ws	-1.60		Cheméo Relay (1.0)
logp	0.652		Crippen Method
mcvol	106.480	ml/mol	McGowan Method
pc	3763.78	kPa	Joback Method
rinpol	1149.30		NIST Webbook
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tb	473.76	K	Cheméo Relay (1.0)
tc	664.90	K	Cheméo Relay (1.0)
tf	289.20	K	Cheméo Relay (1.0)
vc	0.373	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=C24066828&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume