Diethyl 2-isothiocyanatoglutarate

Other names:	2-Isothiocyanato-pentanedioic acid diethyl ester
	Glutaric acid, 2-isothiocyanato-, diethyl ester
Inchi:	InChI=1S/C10H15NO4S/c1-3-14-9(12)6-5-8(11-7-16)10(13)15-4-2/h8H,3-6H2,1-2H3
InchiKey:	BEIMBFWLTYKYLU-UHFFFAOYSA-N
Formula:	C10H15NO4S
SMILES:	CCOC(=O)CCC(N=C=S)C(=O)OCC
Mol. weight [g/mol]:	245.29
CAS:	58560-28-4

Physical Properties

Property code	Value	Unit	Source
hf	-460.54	kJ/mol	Joback Method
hvap	66.22	kJ/mol	Joback Method
log10ws	-1.78		Crippen Method
logp	1.364		Crippen Method
mcvol	184.370	ml/mol	McGowan Method
pc	2365.67	kPa	Joback Method
rinpol	1659.60		NIST Webbook
rinpol	1659.60		NIST Webbook
tb	726.29	K	Joback Method
tc	941.32	K	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C58560284&Units=SI

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