

2-Isothiocyanato-succinic acid diethyl ester

Inchi:	InChI=1S/C9H13NO4S/c1-3-13-8(11)5-7(10-6-15)9(12)14-4-2/h7H,3-5H2,1-2H3
InchiKey:	QXDWIJBRSJSJQ-UHFFFAOYSA-N
Formula:	C9H13NO4S
SMILES:	CCOC(=O)CC(N=C=S)C(=O)OCC
Mol. weight [g/mol]:	231.27

Physical Properties

Property code	Value	Unit	Source
hf	-439.90	kJ/mol	Joback Method
hvap	63.99	kJ/mol	Joback Method
log10ws	-1.36		Crippen Method
logp	0.974		Crippen Method
mcvol	170.280	ml/mol	McGowan Method
pc	2603.08	kPa	Joback Method
rinpol	1527.60		NIST Webbook
tb	703.41	K	Joback Method
tc	921.70	K	Joback Method

Sources

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=R177290&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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