Dimethyl isothiocyanatosuccinate

Inchi:	InChI=1S/C7H9NO4S/c1-11-6(9)3-5(8-4-13)7(10)12-2/h5H,3H2,1-2H3
InchiKey:	NWHDEBYHAZNXDQ-UHFFFAOYSA-N
Formula:	C7H9NO4S
SMILES:	COC(=O)CC(N=C=S)C(=O)OC
Mol. weight [g/mol]:	203.22
CAS:	121928-38-9

Physical Properties

Property code	Value	Unit	Source
hf	-398.62	kJ/mol	Joback Method
hvap	59.54	kJ/mol	Joback Method
log10ws	-0.52		Crippen Method
logp	0.194		Crippen Method
mcvol	142.100	ml/mol	McGowan Method
pc	3199.16	kPa	Joback Method
tb	657.65	K	Joback Method
tc	883.67	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C121928389&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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