

Diethyl isocyanato succinate

Inchi: InChI=1S/C9H13NO5/c1-3-14-8(12)5-7(10-6-11)9(13)15-4-2/h7H,3-5H2,1-2H3
InchiKey: GQPSHLZKDVRQFJ-UHFFFAOYSA-N
Formula: C9H13NO5
SMILES: CCOC(=O)CC(N=C=O)C(=O)OCC
Mol. weight [g/mol]: 215.20
CAS: 17046-24-1

Physical Properties

Property code	Value	Unit	Source
hf	-729.38	kJ/mol	Joback Method
hvap	63.08	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	0.207		Crippen Method
mcvol	159.800	ml/mol	McGowan Method
pc	2746.90	kPa	Joback Method
tb	624.13	K	Joback Method
tc	816.63	K	Joback Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=C17046241&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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