

Ethyl 2-isocyanato-4-methyl valerate

Inchi: InChI=1S/C9H15NO3/c1-4-13-9(12)8(10-6-11)5-7(2)3/h7-8H,4-5H2,1-3H3
InchiKey: SSTQICMSRVMLQN-UHFFFAOYSA-N
Formula: C9H15NO3
SMILES: CCOC(=O)C(CC(C)C)N=C=O
Mol. weight [g/mol]: 185.22
CAS: 64505-10-8

Physical Properties

Property code	Value	Unit	Source
hf	-489.86	kJ/mol	Joback Method
hvap	53.54	kJ/mol	Joback Method
log10ws	-5.82		Crippen Method
logp	1.300		Crippen Method
mcvol	152.360	ml/mol	McGowan Method
pc	2640.67	kPa	Joback Method
tb	547.40	K	Joback Method
tc	737.14	K	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C64505108&Units=SI>
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>

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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