

C4H7NO3S

Inchi: InChI=1S/C4H7NO3S/c1-3(6)4(5-7)9(2)8/h7H,1-2H3/b5-4-
InchiKey: NJGJAXFADDEVOI-PLNGDYQASA-N
Formula: C4H7NO3S
SMILES: CC(=O)C(=NO)S(C)=O
Mol. weight [g/mol]: 149.17
CAS: 112740-56-4

Physical Properties

Property code	Value	Unit	Source
hf	-524.01	kJ/mol	Joback Method
hvap	64.04	kJ/mol	Joback Method
log10ws	1.27		Crippen Method
logp	-0.258		Crippen Method
mcpvol	102.560	ml/mol	McGowan Method
pc	4684.89	kPa	Joback Method
tb	571.81	K	Joback Method
tc	773.68	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C112740564&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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