

C4H7NO2S

Inchi: InChI=1S/C4H7NO2S/c1-3(6)4(5-7)8-2/h7H,1-2H3/b5-4-
InchiKey: LWKWIPSRFUFNQT-PLNGDYQASA-N
Formula: C4H7NO2S
SMILES: CSC(=NO)C(C)=O
Mol. weight [g/mol]: 133.17
CAS: 112740-61-1

Physical Properties

Property code	Value	Unit	Source
hf	-276.40	kJ/mol	Joback Method
hvap	58.13	kJ/mol	Joback Method
log10ws	0.03		Crippen Method
logp	0.726		Crippen Method
mvol	96.690	ml/mol	McGowan Method
pc	4271.86	kPa	Joback Method
tb	582.31	K	Joback Method
tc	796.70	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=C112740611&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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