

C(CH3)2

Inchi:	InChI=1S/C3H6/c1-3-2/h1-2H3
InchiKey:	IPZJQDSFZGZEOY-UHFFFAOYSA-N
Formula:	C3H6
SMILES:	C[C]C
Mol. weight [g/mol]:	42.08
CAS:	40852-89-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.64		Crippen Method
logp	1.107		Crippen Method
mcvol	48.830	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C40852899&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/70-082-3/C-CH3-2.pdf>

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