

(Z)-CH₃CH=CHCH₂COOH

Other names:	cis-Beta,gamma-penteneoic acid
Inchi:	InChI=1S/C5H8O2/c1-2-3-4-5(6)7/h2-3H,4H2,1H3,(H,6,7)/b3-2-
InchiKey:	UIUWNILCHFBLEQ-IHWYPQMZSA-N
Formula:	C5H8O2
SMILES:	CC=CCC([O])=O
Mol. weight [g/mol]:	100.12
CAS:	33698-87-2

Physical Properties

Property code	Value	Unit	Source
chl	-4034.00	kJ/mol	NIST Webbook
log10ws	-5.44		Crippen Method
logp	0.910		Crippen Method
mcvol	82.300	ml/mol	McGowan Method
pc	3878.66 ± 100.00	kPa	NIST Webbook
tc	646.87 ± 3.00	K	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33698872&Units=SI
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

Legend

chl:	Standard liquid enthalpy of combustion
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure

tc: Critical Temperature

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