

«gamma»-campholenic acid methyl ester

Inchi:	InChI=1S/C11H18O2/c1-8-5-6-9(11(8,2)3)7-10(12)13-4/h5,9H,6-7H2,1-4H3
InchiKey:	CKBPZQNPZFCMDU-UHFFFAOYSA-N
Formula:	C11H18O2
SMILES:	<chem>COC(=O)CC1CC=C(C)C1(C)C</chem>
Mol. weight [g/mol]:	182.26

Physical Properties

Property code	Value	Unit	Source
hfus	16.57	kJ/mol	Joback Method
logp	2.542		Crippen Method
mcvol	158.130	ml/mol	McGowan Method
rinpol	1180.00		NIST Webbook
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Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	385.13	J/mol×K	542.36	Joback Method
cpg	401.53	J/mol×K	576.70	Joback Method
cpg	417.06	J/mol×K	611.04	Joback Method
cpg	431.78	J/mol×K	645.38	Joback Method
cpg	445.79	J/mol×K	679.72	Joback Method
cpg	459.17	J/mol×K	714.06	Joback Method
cpg	472.00	J/mol×K	748.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R322202&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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