Methyl-«gamma»-Campholenate

Inchi: InChI=1S/C11H18O2/c1-8-5-6-9(11(8,2)3)7-10(12)13-4/h9H,1,5-7H2,2-4H3
InchiKey: SEXMCXRIYSCDBX-UHFFFAOYSA-N
Formula: C11H18O2
SMILES: C=C1CCC(CC(=O)OC)C1(C)C
Mol. weight [g/mol]: 182.26

Physical Properties

Property code	Value	Unit	Source
gf	-115.75	kJ/mol	Joback Method
hf	-375.55	kJ/mol	Joback Method
hfus	14.58	kJ/mol	Joback Method
hvap	48.19	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	2.542		Crippen Method
mcvol	158.130	ml/mol	McGowan Method
pc	2458.04	kPa	Joback Method
rinpol	1193.00		NIST Webbook
tb	537.38	K	Joback Method
tc	742.15	K	Joback Method
tf	330.13	K	Joback Method
vc	0.598	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	384.14	J/mol×K	537.38	Joback Method
cpg	400.73	J/mol×K	571.51	Joback Method
cpg	416.42	J/mol×K	605.64	Joback Method
cpg	431.32	J/mol×K	639.76	Joback Method
cpg	445.48	J/mol×K	673.89	Joback Method
cpg	459.00	J/mol×K	708.02	Joback Method
cpg	471.95	J/mol×K	742.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R229262&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume