

Methyl-«gamma»-Campholytate

Inchi:	InChI=1S/C10H16O2/c1-7-5-6-8(9(11)12-4)10(7,2)3/h8H,1,5-6H2,2-4H3
InchiKey:	DFUPBVAJURBRBZ-UHFFFAOYSA-N
Formula:	C10H16O2
SMILES:	C=C1CCC(C(=O)OC)C1(C)C
Mol. weight [g/mol]:	168.23

Physical Properties

Property code	Value	Unit	Source
gf	-124.17	kJ/mol	Joback Method
hf	-354.91	kJ/mol	Joback Method
hfus	11.99	kJ/mol	Joback Method
hvap	45.97	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	2.152		Crippen Method
mcvol	144.040	ml/mol	McGowan Method
pc	2709.85	kPa	Joback Method
rinpol	1077.00		NIST Webbook
rinpol	1077.00		NIST Webbook
rinpol	1072.00		NIST Webbook
rinpol	1072.00		NIST Webbook
tb	514.50	K	Joback Method
tc	722.39	K	Joback Method
tf	318.86	K	Joback Method
vc	0.541	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	337.30	J/mol×K	514.50	Joback Method
cpg	353.14	J/mol×K	549.15	Joback Method
cpg	368.10	J/mol×K	583.80	Joback Method
cpg	382.25	J/mol×K	618.45	Joback Method
cpg	395.68	J/mol×K	653.09	Joback Method
cpg	408.47	J/mol×K	687.74	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=R229277&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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