Methyl-«alpha»-Campholytate

Inchi: InChI=1S/C10H16O2/c1-7-5-6-8(9(11)12-4)10(7,2)3/h5,8H,6H2,1-4H3
InchiKey: HLOKTALAKNKDBK-UHFFFAOYSA-N
Formula: C10H16O2
SMILES: COC(=O)C1CC=C(C)C1(C)C
Mol. weight [g/mol]: 168.23

Physical Properties

Property code	Value	Unit	Source
gf	-156.92	kJ/mol	Joback Method
hf	-392.84	kJ/mol	Joback Method
hfus	13.98	kJ/mol	Joback Method
hvap	46.76	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	2.152		Crippen Method
mcvol	144.040	ml/mol	McGowan Method
pc	2715.50	kPa	Joback Method
rinpol	1117.00		NIST Webbook
rinpol	1105.00		NIST Webbook
rinpol	1117.00		NIST Webbook
rinpol	1105.00		NIST Webbook
tb	519.48	K	Joback Method
tc	728.72	K	Joback Method
tf	318.46	K	Joback Method
vc	0.543	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.24	J/mol×K	519.48	Joback Method
cpg	353.90	J/mol×K	554.35	Joback Method
cpg	368.68	J/mol×K	589.23	Joback Method
cpg	382.66	J/mol×K	624.10	Joback Method
cpg	395.93	J/mol×K	658.97	Joback Method
cpg	408.58	J/mol×K	693.85	Joback Method

cpg	420.68	J/mol×K	728.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R229242&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

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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