«alpha»-Campholenic acid

Inchi: InChI=1S/C10H16O2/c1-7-4-5-8(6-9(11)12)10(7,2)3/h4,8H,5-6H2,1-3H3,(H,11,12)
InchiKey: RKLDHGIEBMSKAK-UHFFFAOYSA-N
Formula: C10H16O2
SMILES: CC1=CCC(CC(=O)O)C1(C)C
Mol. weight [g/mol]: 168.23

Physical Properties

Property code	Value	Unit	Source
gf	-188.74	kJ/mol	Joback Method
hf	-412.85	kJ/mol	Joback Method
hfus	16.88	kJ/mol	Joback Method
hvap	61.03	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	2.454		Crippen Method
mcvol	144.040	ml/mol	McGowan Method
pc	3052.41	kPa	Joback Method
rinpol	1277.00		NIST Webbook
rinpol	1277.00		NIST Webbook
ripol	2310.00		NIST Webbook
ripol	2310.00		NIST Webbook
tb	589.24	K	Joback Method
tc	786.65	K	Joback Method
tf	357.05	K	Joback Method
vc	0.544	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	369.86	J/mol×K	589.24	Joback Method
cpg	382.97	J/mol×K	622.14	Joback Method
cpg	395.40	J/mol×K	655.04	Joback Method
cpg	407.23	J/mol×K	687.94	Joback Method
cpg	418.55	J/mol×K	720.85	Joback Method
cpg	429.44	J/mol×K	753.75	Joback Method

cpg	439.99	J/mol×K	786.65	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=R229455&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume