D-Campholic acid

Inchi: InChI=1S/C10H18O2/c1-7-5-6-10(4,8(11)12)9(7,2)3/h7H,5-6H2,1-4H3,(H,11,12)
InchiKey: JDFOIACPOPEQLS-UHFFFAOYSA-N
Formula: C10H18O2
SMILES: CC1CCC(C)(C(=O)O)C1(C)C
Mol. weight [g/mol]: 170.25
CAS: 31147-56-5

Physical Properties

Property code	Value	Unit	Source
gf	-222.27	kJ/mol	Joback Method
hf	-464.26	kJ/mol	Joback Method
hfus	10.82	kJ/mol	Joback Method
hvap	58.62	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	2.533		Crippen Method
mcvol	148.340	ml/mol	McGowan Method
pc	3022.28	kPa	Joback Method
tb	580.67	K	Joback Method
tc	782.51	K	Joback Method
tf	363.43	K	Joback Method
vc	0.555	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	390.46	J/mol×K	580.67	Joback Method
cpg	404.95	J/mol×K	614.31	Joback Method
cpg	418.65	J/mol×K	647.95	Joback Method
cpg	431.73	J/mol×K	681.59	Joback Method
cpg	444.34	J/mol×K	715.23	Joback Method
cpg	456.64	J/mol×K	748.87	Joback Method
cpg	468.78	J/mol×K	782.51	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C31147565&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume