l-camphoronic acid

Inchi: InChI=1S/C9H14O6/c1-8(2,6(12)13)9(3,7(14)15)4-5(10)11/h4H2,1-3H3,(H,10,11)(H,12,1
InchiKey: MJCJFUJXVGIUOD-UHFFFAOYSA-N
Formula: C9H14O6
SMILES: CC(C)(C(=O)O)C(C)(CC(=O)O)C(=O)O
Mol. weight [g/mol]: 218.21

Physical Properties

Property code	Value	Unit	Source
gf	-766.64	kJ/mol	Joback Method
hf	-1041.02	kJ/mol	Joback Method
hfus	21.30	kJ/mol	Joback Method
hvap	103.31	kJ/mol	Joback Method
log10ws	-0.29		Aqueous Solubility Prediction Method
logp	0.663		Crippen Method
mcvol	159.990	ml/mol	McGowan Method
pc	4010.84	kPa	Joback Method
tb	837.01	K	Joback Method
tc	1031.21	K	Joback Method
tf	528.28	K	Joback Method
vc	0.593	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	478.50	J/mol×K	837.01	Joback Method
cpg	485.48	J/mol×K	869.38	Joback Method
cpg	492.03	J/mol×K	901.74	Joback Method
cpg	498.17	J/mol×K	934.11	Joback Method
cpg	503.96	J/mol×K	966.47	Joback Method
cpg	509.46	J/mol×K	998.84	Joback Method
cpg	514.70	J/mol×K	1031.21	Joback Method
dvisc	0.0002007	Pa×s	528.28	Joback Method
dvisc	0.0000566	Pa×s	579.74	Joback Method

dvisc	0.0000196	Pa×s	631.19	Joback Method
dvisc	0.0000080	Pa×s	682.64	Joback Method
dvisc	0.0000037	Pa×s	734.10	Joback Method
dvisc	0.0000019	Pa×s	785.56	Joback Method
dvisc	0.0000010	Pa×s	837.01	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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