2-(4-Methyl-2-oxo-cyclohexyl)-propanoic acid

Inchi: InChI=1S/C10H16O3/c1-6-3-4-8(9(11)5-6)7(2)10(12)13/h6-8H,3-5H2,1-2H3,(H,12,13)
InchiKey: NLVKRMKUKIWVJS-UHFFFAOYSA-N
Formula: C10H16O3
SMILES: CC1CCC(C(C)C(=O)O)C(=O)C1
Mol. weight [g/mol]: 184.23

Physical Properties

Property code	Value	Unit	Source
gf	-340.71	kJ/mol	Joback Method
hf	-623.54	kJ/mol	Joback Method
hfus	16.24	kJ/mol	Joback Method
hvap	65.26	kJ/mol	Joback Method
log10ws	-1.56		Crippen Method
logp	1.712		Crippen Method
mcvol	149.910	ml/mol	McGowan Method
pc	3059.17	kPa	Joback Method
ripol	2820.00		NIST Webbook
ripol	2820.00		NIST Webbook
tb	656.51	K	Joback Method
tc	866.39	K	Joback Method
tf	369.57	K	Joback Method
vc	0.553	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	424.66	J/mol×K	656.51	Joback Method
cpg	439.84	J/mol×K	691.49	Joback Method
cpg	454.13	J/mol×K	726.47	Joback Method
cpg	467.52	J/mol×K	761.45	Joback Method
cpg	480.00	J/mol×K	796.43	Joback Method
cpg	491.57	J/mol×K	831.41	Joback Method
cpg	502.22	J/mol×K	866.39	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R326091&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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