Cyclohexanepropionic acid, 4,4-dimethyl-2,6-dioxo-

Inchi: InChI=1S/C11H16O4/c1-11(2)5-8(12)7(9(13)6-11)3-4-10(14)15/h12H,3-6H2,1-2H3,(H,14

InchiKey: CLECEIACDNHONJ-UHFFFAOYSA-N

Formula: C11H16O4

SMILES: CC1(C)CC(=O)C(CCC(=O)O)=C(O)C1

Mol. weight [g/mol]: 212.24

Physical Properties

Property code	Value	Unit	Source
gf	-453.75	kJ/mol	Joback Method
hf	-720.71	kJ/mol	Joback Method
hfus	19.51	kJ/mol	Joback Method
hvap	85.33	kJ/mol	Joback Method
log10ws	-2.13		Crippen Method
logp	2.052		Crippen Method
mcvol	165.570	ml/mol	McGowan Method
pc	3318.18	kPa	Joback Method
tb	786.04	K	Joback Method
tc	989.26	K	Joback Method
tf	510.60	K	Joback Method
vc	0.620	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.42	J/mol×K	786.04	Joback Method
cpg	508.33	J/mol×K	819.91	Joback Method
cpg	519.89	J/mol×K	853.78	Joback Method
cpg	531.16	J/mol×K	887.65	Joback Method
cpg	542.21	J/mol×K	921.52	Joback Method
cpg	553.11	J/mol×K	955.39	Joback Method
cpg	563.92	J/mol×K	989.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6007907&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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