Cyclohexanevaleric acid, 4,4-dimethyl-d,2,6-trioxo-

Inchi: InChI=1S/C13H18O5/c1-13(2)6-9(15)12(10(16)7-13)8(14)4-3-5-11(17)18/h12H,3-7H2,1-
InchiKey: UDRPIGWMAPUXKP-UHFFFAOYSA-N
Formula: C13H18O5
SMILES: CC1(C)CC(=O)C(C(=O)CCCC(=O)O)C(=O)C1
Mol. weight [g/mol]: 254.28

Physical Properties

Property code	Value	Unit	Source
gf	-570.01	kJ/mol	Joback Method
hf	-915.22	kJ/mol	Joback Method
hfus	22.34	kJ/mol	Joback Method
hvap	82.17	kJ/mol	Joback Method
log10ws	-1.62		Crippen Method
logp	1.385		Crippen Method
mcvol	195.320	ml/mol	McGowan Method
pc	2600.43	kPa	Joback Method
tb	847.52	K	Joback Method
tc	1068.75	K	Joback Method
tf	560.43	K	Joback Method
vc	0.739	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	627.27	J/mol×K	847.52	Joback Method
cpg	641.98	J/mol×K	884.39	Joback Method
cpg	656.03	J/mol×K	921.26	Joback Method
cpg	669.46	J/mol×K	958.14	Joback Method
cpg	682.34	J/mol×K	995.01	Joback Method
cpg	694.72	J/mol×K	1031.88	Joback Method
cpg	706.65	J/mol×K	1068.75	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=B6007383&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