Cyclohexanepropionamide, 4,4-dimethyl-2,6-dioxo-

Inchi: InChI=1S/C11H17NO3/c1-11(2)5-8(13)7(9(14)6-11)3-4-10(12)15/h7H,3-6H2,1-2H3,(H2,1

InchiKey: AMKUXQLBNFMVBI-UHFFFAOYSA-N

Formula: C11H17NO3

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

Mol. weight [g/mol]: 211.26

CAS: 116594-63-9

Physical Properties

Property code	Value	Unit	Source
gf	-125.41	kJ/mol	Joback Method
hf	-450.45	kJ/mol	Joback Method
hvap	76.30	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	1.876		Crippen Method
mcvol	169.680	ml/mol	McGowan Method
tb	778.36	K	Joback Method
tf	506.81	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	530.75	J/mol×K	778.36	Joback Method
cpg	56.52	J/mol×K	100.12	Joback Method
cpg	56.52	J/mol×K	100.12	Joback Method
cpg	56.52	J/mol×K	100.12	Joback Method
cpg	56.52	J/mol×K	100.12	Joback Method
cpg	56.52	J/mol×K	100.12	Joback Method
cpg	56.52	J/mol×K	100.12	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116594639&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation 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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point