(7,7-Dimethyl-1,4-dioxo-2,3,4,5,6,7-hexahydro-1H-
acid

Inchi: InChI=1S/C13H16O4/c1-13(2)4-3-9(14)8-5-7(6-10(15)16)12(17)11(8)13/h7H,3-6H2,1-2H

InchiKey: UDGQJBVBTOPBIQ-UHFFFAOYSA-N

Formula: C13H16O4

SMILES: CC1(C)CCC(=O)C2=C1C(=O)C(CC(=O)O)C2

Mol. weight [g/mol]: 236.26

CAS: 59488-99-2

Physical Properties

Property code	Value	Unit	Source
gf	-361.93	kJ/mol	Joback Method
hf	-674.66	kJ/mol	Joback Method
hfus	18.25	kJ/mol	Joback Method
hvap	77.26	kJ/mol	Joback Method
log10ws	-2.08		Crippen Method
logp	1.736		Crippen Method
mcvol	178.590	ml/mol	McGowan Method
pc	2906.11	kPa	Joback Method
rinpol	1977.00		NIST Webbook
rinpol	1977.00		NIST Webbook
tb	814.18	K	Joback Method
tc	1043.64	K	Joback Method
tf	558.48	K	Joback Method
vc	0.676	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	562.23	J/mol×K	814.18	Joback Method
cpg	577.17	J/mol×K	852.42	Joback Method
cpg	591.58	J/mol×K	890.67	Joback Method
cpg	605.56	J/mol×K	928.91	Joback Method
cpg	619.20	J/mol×K	967.15	Joback Method
cpg	632.60	J/mol×K	1005.40	Joback Method
cpg	645.85	J/mol×K	1043.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C59488992&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume