1-(1,2,2-Trimethylcyclopent-1-yl)-pentan-1,4-dione

Inchi: InChI=1S/C13H22O2/c1-10(14)6-7-11(15)13(4)9-5-8-12(13,2)3/h5-9H2,1-4H3
InchiKey: XKYXMUWTRPUUIL-UHFFFAOYSA-N
Formula: C13H22O2
SMILES: CC(=O)CCC(=O)C1(C)CCCC1(C)C
Mol. weight [g/mol]: 210.31

Physical Properties

Property code	Value	Unit	Source
gf	-181.40	kJ/mol	Joback Method
hf	-466.19	kJ/mol	Joback Method
hfus	15.03	kJ/mol	Joback Method
hvap	55.67	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	3.141		Crippen Method
mcvol	186.310	ml/mol	McGowan Method
pc	2261.11	kPa	Joback Method
rinpol	1492.00		NIST Webbook
rinpol	1492.00		NIST Webbook
tb	615.67	K	Joback Method
tc	829.98	K	Joback Method
tf	390.59	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.80	J/mol×K	615.67	Joback Method
cpg	516.47	J/mol×K	651.39	Joback Method
cpg	533.26	J/mol×K	687.11	Joback Method
cpg	549.34	J/mol×K	722.83	Joback Method
cpg	564.93	J/mol×K	758.55	Joback Method
cpg	580.23	J/mol×K	794.27	Joback Method
cpg	595.43	J/mol×K	829.98	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=R229099&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume