2-Pentene-1,4-dione, 1-(1,2,2-trimethylcyclopentyl)

Other names: (1,2,2-trimethyl-l-cyclopentyl)-2-pentene- 1,4-dione
Inchi: InChI=1S/C13H20O2/c1-10(14)6-7-11(15)13(4)9-5-8-12(13,2)3/h6-7H,5,8-9H2,1-4H3/b7-
InchiKey: OEAWUKBLZBMTNY-SREVYHEPSA-N
Formula: C13H20O2
SMILES: CC(=O)C=CC(=O)C1(C)CCCC1(C)C
Mol. weight [g/mol]: 208.30

Physical Properties

Property code	Value	Unit	Source
gf	-101.18	kJ/mol	Joback Method
hf	-348.97	kJ/mol	Joback Method
hfus	15.24	kJ/mol	Joback Method
hvap	55.63	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	2.917		Crippen Method
mcvol	182.010	ml/mol	McGowan Method
pc	2377.22	kPa	Joback Method
ripol	2111.00		NIST Webbook
ripol	2176.00		NIST Webbook
ripol	2111.00		NIST Webbook
tb	619.83	K	Joback Method
tc	843.23	K	Joback Method
tf	385.51	K	Joback Method
vc	0.692	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	478.21	J/mol×K	619.83	Joback Method
cpg	495.42	J/mol×K	657.06	Joback Method
cpg	511.72	J/mol×K	694.30	Joback Method
cpg	527.34	J/mol×K	731.53	Joback Method
cpg	542.53	J/mol×K	768.76	Joback Method
cpg	557.54	J/mol×K	806.00	Joback Method

cpg	572.60	J/mol×K	843.23	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=U196779&Units=SI

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume