2-Cyclohexen-1-one, 3,5,5-trimethyl-4-(3-oxo-1-butynyl)

Other names: 4-(3-Oxo-1-butynyl)-3,5,5-trimethyl-cyclohex-2-en-1-one
Inchi: InChI=1S/C13H16O2/c1-9-7-11(15)8-13(3,4)12(9)6-5-10(2)14/h7,12H,8H2,1-4H3
InchiKey: WWUPVQPXAIQTFK-UHFFFAOYSA-N
Formula: C13H16O2
SMILES: CC(=O)C#CC1C(C)=CC(=O)CC1(C)C
Mol. weight [g/mol]: 204.26

Physical Properties

Property code	Value	Unit	Source
gf	41.45	kJ/mol	Joback Method
hf	-194.10	kJ/mol	Joback Method
hfus	21.10	kJ/mol	Joback Method
hvap	57.60	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.140		Crippen Method
mcvol	173.410	ml/mol	McGowan Method
pc	2576.72	kPa	Joback Method
rinpol	1452.00		NIST Webbook
rinpol	1475.00		NIST Webbook
rinpol	1474.00		NIST Webbook
tb	646.79	K	Joback Method
tc	894.99	K	Joback Method
tf	500.84	K	Joback Method
vc	0.654	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	450.73	J/mol×K	646.79	Joback Method
cpg	468.68	J/mol×K	688.16	Joback Method
cpg	485.70	J/mol×K	729.52	Joback Method
cpg	501.90	J/mol×K	770.89	Joback Method
cpg	517.38	J/mol×K	812.26	Joback Method
cpg	532.27	J/mol×K	853.62	Joback Method

cpg	546.67	J/mol×K	894.99	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=R194988&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