2-Buten-1-one, 1-(2,6,6-trimethyl-1-cyclohexen-1-yl)-

Other names: 1-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-2-buten-1-one
2,6,6-Trimethyl-1-crotonoyl-1-cyclohexene
Damascone

Inchi: InChI=1S/C13H20O/c1-5-7-11(14)12-10(2)8-6-9-13(12,3)4/h5,7H,6,8-9H2,1-4H3/b7-5+

InchiKey: BGTBFNDXYDYBEY-FNORWQNLSA-N

Formula: C13H20O

SMILES: CC=CC(=O)C1=C(C)CCCC1(C)C

Mol. weight [g/mol]: 192.30

CAS: 35044-68-9

Physical Properties

Property code	Value	Unit	Source
gf	39.54	kJ/mol	Joback Method
hf	-202.61	kJ/mol	Joback Method
hfus	17.21	kJ/mol	Joback Method
hvap	52.13	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.658		Crippen Method
mcvol	176.140	ml/mol	McGowan Method
pc	2278.41	kPa	Joback Method
rinpol	1366.80		NIST Webbook
rinpol	1456.00		NIST Webbook
rinpol	1392.00		NIST Webbook
rinpol	1419.30		NIST Webbook
rinpol	1415.00		NIST Webbook
rinpol	1411.00		NIST Webbook
rinpol	1419.00		NIST Webbook
rinpol	1420.00		NIST Webbook
rinpol	1422.00		NIST Webbook
rinpol	1431.00		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1391.60		NIST Webbook
rinpol	1401.00		NIST Webbook
rinpol	1412.00		NIST Webbook
rinpol	1394.00		NIST Webbook
rinpol	1395.00		NIST Webbook
rinpol	1400.00		NIST Webbook

rinpol	1406.00		NIST Webbook
rinpol	1408.00		NIST Webbook
rinpol	1391.60		NIST Webbook
rinpol	1393.00		NIST Webbook
rinpol	1409.00		NIST Webbook
rinpol	1403.00		NIST Webbook
rinpol	1383.00		NIST Webbook
rinpol	1401.00		NIST Webbook
rinpol	1366.60		NIST Webbook
rinpol	1431.00		NIST Webbook
ripol	1797.00		NIST Webbook
ripol	1782.00		NIST Webbook
ripol	1836.00		NIST Webbook
ripol	1797.00		NIST Webbook
ripol	1830.00		NIST Webbook
ripol	1836.00		NIST Webbook
ripol	1830.00		NIST Webbook
ripol	1830.00		NIST Webbook
ripol	1815.00		NIST Webbook
ripol	1830.00		NIST Webbook
ripol	1822.00		NIST Webbook
ripol	1824.00		NIST Webbook
ripol	1830.00		NIST Webbook
ripol	1830.00		NIST Webbook
tb	583.78	K	Joback Method
tc	802.88	K	Joback Method
tf	338.20	K	Joback Method
vc	0.666	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.25	J/mol×K	583.78	Joback Method
cpg	455.12	J/mol×K	620.30	Joback Method
cpg	471.95	J/mol×K	656.81	Joback Method
cpg	487.87	J/mol×K	693.33	Joback Method
cpg	503.02	J/mol×K	729.85	Joback Method
cpg	517.51	J/mol×K	766.36	Joback Method
cpg	531.49	J/mol×K	802.88	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=C35044689&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume