2-methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-2-b

Other names: 2-Butenal, 2-methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-
Inchi: InChI=1S/C14H22O/c1-11(10-15)7-8-13-12(2)6-5-9-14(13,3)4/h6-7,10,13H,5,8-9H2,1-4H
InchiKey: JJHZLPJQTHPGEI-UHFFFAOYSA-N
Formula: C14H22O
SMILES: CC(C=O)=CCC1C(C)=CCCC1(C)C
Mol. weight [g/mol]: 206.32
CAS: 68555-62-4

Physical Properties

Property code	Value	Unit	Source
chl	-8420.70 ± 2.30	kJ/mol	NIST Webbook
gf	70.73	kJ/mol	Joback Method
hf	-214.91	kJ/mol	Joback Method
hfl	227.20 ± 2.30	kJ/mol	NIST Webbook
hfus	20.64	kJ/mol	Joback Method
hvap	53.44	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	3.904		Crippen Method
mcvol	190.230	ml/mol	McGowan Method
pc	2079.33	kPa	Joback Method
tb	591.68	K	Joback Method
tc	804.87	K	Joback Method
tf	310.82	K	Joback Method
vc	0.734	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	489.02	J/mol×K	591.68	Joback Method
cpg	508.04	J/mol×K	627.21	Joback Method
cpg	525.99	J/mol×K	662.74	Joback Method
cpg	542.98	J/mol×K	698.28	Joback Method
cpg	559.14	J/mol×K	733.81	Joback Method
cpg	574.59	J/mol×K	769.34	Joback Method

cpg	589.46	J/mol×K	804.87	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C68555624&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume