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

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]: 206.33

Physical Properties

Property code	Value	Unit	Source
chl	-8420.70 ± 2.30	kJ/mol	NIST Webbook
hfl	227.20 ± 2.30	kJ/mol	NIST Webbook
hfus	20.64	kJ/mol	Joback Method
logp	3.904		Crippen Method
mcvol	190.230	ml/mol	McGowan 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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C68555624&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume