2-HYDROXY-3,5,5-TRIMETHYL-CYCLOHEX-2-ENO

Other names:	2-Hydroxy-3,5,5-trimethyl-2-cyclohexen-1-one
	2-Hydroxyisophorone
	2-Cyclohexen-1-one, 2-hydroxy-3,5,5-trimethyl-
Inchi:	InChI=1S/C9H14O2/c1-6-4-9(2,3)5-7(10)8(6)11/h11H,4-5H2,1-3H3
InchiKey:	DWGZTTFGUFHAJX-UHFFFAOYSA-N
Formula:	C9H14O2
SMILES:	CC1=C(O)C(=O)CC(C)(C)C1
Mol. weight [g/mol]:	154.21

Physical Properties

Property code	Value	Unit	Source
hfus	8.64	kJ/mol	Joback Method
ie	8.82	eV	Cheméo Relay (1.0)
logp	2.208		Crippen Method
mcvol	129.950	ml/mol	McGowan Method
rinpol	1149.80		NIST Webbook
rinpol	1194.00		NIST Webbook
ripol	1675.00		NIST Webbook
ripol	1648.00		NIST Webbook
ripol	1675.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	329.34	J/mol×K	594.23	Joback Method
cpg	342.50	J/mol×K	629.82	Joback Method
cpg	355.06	J/mol×K	665.41	Joback Method
cpg	367.09	J/mol×K	701.00	Joback Method
cpg	378.65	J/mol×K	736.59	Joback Method
cpg	389.81	J/mol×K	772.18	Joback Method
cpg	400.65	J/mol×K	807.77	Joback Method

Sources

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=C4883607&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices