S-(+)-5-(1-Hydroxy-1-methylethyl)-2-methyl-2-cycl

Other names: 5-(1-Hydroxy-1-methylethyl)-2-methyl-2-cyclohexen-1-one, (S)-
D-8-Hydroxycarvotanacetone
(S)-8-Hydroxy-p-menth-1-en-6-one
Carvone hydrate
Carvon hydrate

Inchi: InChI=1S/C10H16O2/c1-7-4-5-8(6-9(7)11)10(2,3)12/h4,8,12H,5-6H2,1-3H3/t8-/m0/s1

InchiKey: DJOOMNLGIUGRKD-QMMMGPOBSA-N

Formula: C10H16O2

SMILES: CC1=CCC(C(C)(C)O)CC1=O

Mol. weight [g/mol]: 168.23

CAS: 60593-11-5

Physical Properties

Property code	Value	Unit	Source
gf	-178.47	kJ/mol	Joback Method
hf	-447.78	kJ/mol	Joback Method
hfus	10.51	kJ/mol	Joback Method
hvap	58.87	kJ/mol	Joback Method
log10ws	-2.17		Crippen Method
logp	1.683		Crippen Method
mcvol	144.040	ml/mol	McGowan Method
pc	3065.95	kPa	Joback Method
rinpol	1424.00		NIST Webbook
ripol	1754.00		NIST Webbook
tb	608.66	K	Joback Method
tc	822.00	K	Joback Method
tf	354.58	K	Joback Method
vc	0.529	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	384.00	J/mol×K	608.66	Joback Method
cpg	399.22	J/mol×K	644.22	Joback Method

cpg	413.54	J/mol×K	679.77	Joback Method
cpg	426.99	J/mol×K	715.33	Joback Method
cpg	439.59	J/mol×K	750.88	Joback Method
cpg	451.34	J/mol×K	786.44	Joback Method
cpg	462.27	J/mol×K	822.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C60593115&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

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