5-Hepten-3-one, 2-(5-ethenyltetrahydro-5-methyl-2-furanyl)-6-meth [2S-[2«alpha»(R*),5«alpha»]]-

Other names: 5-Hepten-3-one, 6-methyl-2-(tetrahydro-5-methyl-5-vinyl-2-furyl)-, (+)-
Davanone
5-Hepten-3-one, 2-(5-ethenyltetrahydro-5-methyl-2-furanyl)-6-methyl-
5-Hepten-3-one, 6-methyl-2-(tetrahydro-5-methyl-5-vinyl-2-furyl)-

Inchi: InChI=1S/C15H24O2/c1-6-15(5)10-9-14(17-15)12(4)13(16)8-7-11(2)3/h6-7,12,14H,1,8-1

InchiKey: FJKKZNIYYVEYOL-JENMUQSASA-N

Formula: C15H24O2

SMILES: C=CC1(C)CCC(C(C)C(=O)CC=C(C)C)O1

Mol. weight [g/mol]: 236.35

CAS: 20482-11-5

Physical Properties

Property code	Value	Unit	Source
gf	40.80	kJ/mol	Joback Method
hf	-314.55	kJ/mol	Joback Method
hfus	26.98	kJ/mol	Joback Method
hvap	58.02	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	3.672		Crippen Method
mcvol	210.190	ml/mol	McGowan Method
pc	1882.17	kPa	Joback Method
rinpol	1554.00		NIST Webbook
rinpol	1593.00		NIST Webbook
rinpol	1608.00		NIST Webbook
rinpol	1567.00		NIST Webbook
rinpol	1559.00		NIST Webbook
rinpol	1567.00		NIST Webbook
rinpol	1559.00		NIST Webbook
rinpol	1561.00		NIST Webbook
rinpol	1592.00		NIST Webbook
rinpol	1586.00		NIST Webbook
rinpol	1568.00		NIST Webbook
rinpol	1592.00		NIST Webbook
rinpol	1561.00		NIST Webbook
rinpol	1592.00		NIST Webbook
rinpol	1554.00		NIST Webbook
rinpol	1567.00		NIST Webbook

rinpol	1552.00		NIST Webbook
rinpol	1593.00		NIST Webbook
rinpol	1588.00		NIST Webbook
rinpol	1608.00		NIST Webbook
rinpol	1580.00		NIST Webbook
rinpol	1553.00		NIST Webbook
rinpol	1567.00		NIST Webbook
rinpol	1608.00		NIST Webbook
rinpol	1609.00		NIST Webbook
rinpol	1588.00		NIST Webbook
rinpol	1586.00		NIST Webbook
rinpol	1561.00		NIST Webbook
ripol	2040.00		NIST Webbook
ripol	2040.00		NIST Webbook
tb	634.55	K	Joback Method
tc	845.68	K	Joback Method
tf	330.07	K	Joback Method
vc	0.796	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.19	J/mol×K	634.55	Joback Method
cpg	592.37	J/mol×K	669.74	Joback Method
cpg	610.50	J/mol×K	704.93	Joback Method
cpg	627.73	J/mol×K	740.11	Joback Method
cpg	644.19	J/mol×K	775.30	Joback Method
cpg	660.02	J/mol×K	810.49	Joback Method
cpg	675.35	J/mol×K	845.68	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C20482115&Units=SI

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