

4,5-dihydrovomifoliol

Inchi:	InChI=1S/C15H22O4/c1-8-9-4-6-14(2)10(16)5-7-15(3,18)12(14)11(9)19-13(8)17/h8-9,11
InchiKey:	SMEJXMYNQKQENF-UHFFFAOYSA-N
Formula:	C15H22O4
SMILES:	CC1C(=O)OC2C1CCC1(C)C(=O)CCC(C)(O)C21
Mol. weight [g/mol]:	266.33

Physical Properties

Property code	Value	Unit	Source
gf	-292.96	kJ/mol	Joback Method
hf	-749.34	kJ/mol	Joback Method
hfus	22.32	kJ/mol	Joback Method
hvap	75.86	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	1.694		Crippen Method
mcvol	204.510	ml/mol	McGowan Method
pc	2441.06	kPa	Joback Method
ripol	3002.00		NIST Webbook
ripol	3017.00		NIST Webbook
ripol	3002.00		NIST Webbook
ripol	3017.00		NIST Webbook
ripol	3024.00		NIST Webbook
ripol	3064.00		NIST Webbook
ripol	3062.00		NIST Webbook
tb	821.14	K	Joback Method
tc	1058.33	K	Joback Method
tf	557.46	K	Joback Method
vc	0.761	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	715.29	J/mol×K	821.14	Joback Method
cpg	736.36	J/mol×K	860.67	Joback Method
cpg	757.23	J/mol×K	900.20	Joback Method

cpg	778.13	J/mol×K	939.74	Joback Method
cpg	799.31	J/mol×K	979.27	Joback Method
cpg	821.00	J/mol×K	1018.80	Joback Method
cpg	843.43	J/mol×K	1058.33	Joback Method

Sources

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=R302595&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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