

Villosin

Inchi:	InChI=1S/C20H28O2/c1-14-6-9-17-19(2,3)11-5-12-20(17,4)16(14)8-7-15-10-13-22-18(15)
InchiKey:	HVTQZHAAIRBKHO-BQYQJAHWSA-N
Formula:	C20H28O2
SMILES:	<chem>C=C1CCC2C(C)(C)CCCC2(C)C1C=CC1=CCOC1=O</chem>
Mol. weight [g/mol]:	300.44
CAS:	160598-92-5

Physical Properties

Property code	Value	Unit	Source
gf	153.40	kJ/mol	Joback Method
hf	-286.48	kJ/mol	Joback Method
hfus	25.20	kJ/mol	Joback Method
hvap	68.10	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	4.825		Crippen Method
mcvol	254.620	ml/mol	McGowan Method
pc	1703.31	kPa	Joback Method
rinpol	2575.10		NIST Webbook
rinpol	2575.10		NIST Webbook
tb	800.88	K	Joback Method
tc	1051.80	K	Joback Method
tf	508.09	K	Joback Method
vc	0.952	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	824.86	J/mol×K	800.88	Joback Method
cpg	850.08	J/mol×K	842.70	Joback Method
cpg	874.89	J/mol×K	884.52	Joback Method
cpg	899.65	J/mol×K	926.34	Joback Method
cpg	924.69	J/mol×K	968.16	Joback Method
cpg	950.37	J/mol×K	1009.98	Joback Method
cpg	977.04	J/mol×K	1051.80	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=C160598925&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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