

Occidol acetate

Inchi:	InChI=1S/C17H24O2/c1-11-6-7-12(2)16-10-14(8-9-15(11)16)17(4,5)19-13(3)18/h6-7,14H
InchiKey:	JBIUFFGIDNZYFQ-UHFFFAOYSA-N
Formula:	C17H24O2
SMILES:	CC(=O)OC(C)(C)C1CCc2c(C)ccc(C)c2C1
Mol. weight [g/mol]:	260.37
CAS:	61263-48-7

Physical Properties

Property code	Value	Unit	Source
gf	-6.65	kJ/mol	Joback Method
hf	-379.00	kJ/mol	Joback Method
hfus	24.07	kJ/mol	Joback Method
hvap	65.64	kJ/mol	Joback Method
log10ws	-4.75		Crippen Method
logp	3.750		Crippen Method
mvol	223.210	ml/mol	McGowan Method
pc	1820.06	kPa	Joback Method
rinpol	1974.00		NIST Webbook
rinpol	1974.00		NIST Webbook
tb	714.05	K	Joback Method
tc	937.42	K	Joback Method
tf	434.33	K	Joback Method
vc	0.842	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	644.26	J/molxK	714.05	Joback Method
cpg	662.99	J/molxK	751.28	Joback Method
cpg	680.46	J/molxK	788.51	Joback Method
cpg	696.75	J/molxK	825.73	Joback Method
cpg	711.92	J/molxK	862.96	Joback Method
cpg	726.04	J/molxK	900.19	Joback Method
cpg	739.17	J/molxK	937.42	Joback Method

dvisc	0.0011893	Paxs	434.33	Joback Method
dvisc	0.0007448	Paxs	480.95	Joback Method
dvisc	0.0005066	Paxs	527.57	Joback Method
dvisc	0.0003669	Paxs	574.19	Joback Method
dvisc	0.0002789	Paxs	620.81	Joback Method
dvisc	0.0002203	Paxs	667.43	Joback Method
dvisc	0.0001794	Paxs	714.05	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=C61263487&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
mvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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