

3',6'-Diacetoxynorbornadiene

Inchi:	InChI=1S/C15H14O4/c1-8(16)18-12-5-6-13(19-9(2)17)15-11-4-3-10(7-11)14(12)15/h3-6,
InchiKey:	GHNDBDFQIQOER-UHFFFAOYSA-N
Formula:	C15H14O4
SMILES:	CC(=O)Oc1ccc(OC(C)=O)c2c1C1C=CC2C1
Mol. weight [g/mol]:	258.27
CAS:	7213-65-2

Physical Properties

Property code	Value	Unit	Source
gf	-145.34	kJ/mol	Joback Method
hf	-430.87	kJ/mol	Joback Method
hfus	32.65	kJ/mol	Joback Method
hvap	71.50	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	2.678		Crippen Method
mcvol	187.310	ml/mol	McGowan Method
pc	2477.65	kPa	Joback Method
tb	745.17	K	Joback Method
tc	969.93	K	Joback Method
tf	507.27	K	Joback Method
vc	0.724	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	531.28	J/molxK	745.17	Joback Method
cpg	544.63	J/molxK	782.63	Joback Method
cpg	557.10	J/molxK	820.09	Joback Method
cpg	568.76	J/molxK	857.55	Joback Method
cpg	579.69	J/molxK	895.01	Joback Method
cpg	589.95	J/molxK	932.47	Joback Method
cpg	599.61	J/molxK	969.93	Joback Method
dvisc	0.0023670	Paxs	507.27	Joback Method
dvisc	0.0020523	Paxs	546.92	Joback Method

dvisc	0.0018141	Paxs	586.57	Joback Method
dvisc	0.0016288	Paxs	626.22	Joback Method
dvisc	0.0014813	Paxs	665.87	Joback Method
dvisc	0.0013616	Paxs	705.52	Joback Method
dvisc	0.0012629	Paxs	745.17	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=C7213652&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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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