

nothoapiole

Inchi:	InChI=1S/C13H16O5/c1-5-6-8-9(14-2)11(16-4)13-12(10(8)15-3)17-7-18-13/h5H,1,6-7H2
InchiKey:	IWGPXDGGZYMDJF-UHFFFAOYSA-N
Formula:	C13H16O5
SMILES:	<chem>C=CCc1c(OC)c(OC)c2c(c1OC)OCO2</chem>
Mol. weight [g/mol]:	252.26

Physical Properties

Property code	Value	Unit	Source
gf	-208.10	kJ/mol	Joback Method
hf	-574.56	kJ/mol	Joback Method
hfus	36.83	kJ/mol	Joback Method
hvap	65.92	kJ/mol	Joback Method
log10ws	-3.12		Crippen Method
logp	2.170		Crippen Method
mcvol	184.460	ml/mol	McGowan Method
pc	2324.78	kPa	Joback Method
rmpol	1759.00		NIST Webbook
tb	677.67	K	Joback Method
tc	887.81	K	Joback Method
tf	465.54	K	Joback Method
vc	0.691	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	495.95	J/molxK	677.67	Joback Method
cpg	509.76	J/molxK	712.69	Joback Method
cpg	522.84	J/molxK	747.72	Joback Method
cpg	535.18	J/molxK	782.74	Joback Method
cpg	546.78	J/molxK	817.76	Joback Method
cpg	557.65	J/molxK	852.79	Joback Method
cpg	567.79	J/molxK	887.81	Joback Method
dvisc	0.0006519	Paxs	465.54	Joback Method
dvisc	0.0004963	Paxs	500.89	Joback Method

dvisc	0.0003917	Paxs	536.25	Joback Method
dvisc	0.0003183	Paxs	571.61	Joback Method
dvisc	0.0002650	Paxs	606.96	Joback Method
dvisc	0.0002252	Paxs	642.32	Joback Method
dvisc	0.0001946	Paxs	677.67	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=R436381&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
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
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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