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: C=CCc1c(OC)c(OC)c2c(c1OC)OCO2
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
rinpol	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	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0003917	Pa×s	536.25	Joback Method
dvisc	0.0003183	Pa×s	571.61	Joback Method
dvisc	0.0002650	Pa×s	606.96	Joback Method
dvisc	0.0002252	Pa×s	642.32	Joback Method
dvisc	0.0001946	Pa×s	677.67	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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/ci990307l

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
mcvol:	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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