wettstein A

Inchi: InChI=1S/C13H12O4/c1-14-10-8-5-3-4-6-9(8)11-13(12(10)15-2)17-7-16-11/h3-6H,7H2,1-
InchiKey: JRTKQSYUDQVSHV-UHFFFAOYSA-N
Formula: C13H12O4
SMILES: COc1c2c(c3ccccc3c1OC)OCO2
Mol. weight [g/mol]: 232.23
CAS: 74066-35-6

Physical Properties

Property code	Value	Unit	Source
gf	-74.66	kJ/mol	Joback Method
hf	-365.23	kJ/mol	Joback Method
hfus	34.33	kJ/mol	Joback Method
hvap	65.16	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	2.586		Crippen Method
mcvol	163.430	ml/mol	McGowan Method
pc	2956.90	kPa	Joback Method
rinpol	1845.00		NIST Webbook
rinpol	1845.00		NIST Webbook
tb	672.57	K	Joback Method
tc	905.76	K	Joback Method
tf	465.25	K	Joback Method
vc	0.614	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	430.70	J/mol×K	672.57	Joback Method
cpg	443.82	J/mol×K	711.43	Joback Method
cpg	456.06	J/mol×K	750.30	Joback Method
cpg	467.50	J/mol×K	789.16	Joback Method
cpg	478.17	J/mol×K	828.03	Joback Method
cpg	488.14	J/mol×K	866.89	Joback Method
cpg	497.46	J/mol×K	905.76	Joback Method

dvisc	0.0011242	Pa×s	465.25	Joback Method
dvisc	0.0009002	Pa×s	499.80	Joback Method
dvisc	0.0007419	Pa×s	534.36	Joback Method
dvisc	0.0006260	Pa×s	568.91	Joback Method
dvisc	0.0005385	Pa×s	603.46	Joback Method
dvisc	0.0004709	Pa×s	638.02	Joback Method
dvisc	0.0004175	Pa×s	672.57	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C74066356&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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