7-Ethyl-3-methyl-5-propenyl-2-(3,4,5-trimethoxy-p

Inchi: InChI=1S/C23H28O4/c1-7-9-15-10-16(8-2)22-18(11-15)14(3)21(27-22)17-12-19(24-4)23(26-6)20(25-5)13-17/h7,9-10,12-13H,8,11H2,1-6H3/b9-7+
InchiKey: IFKTXFRFKOYFLG-VQHVLOKHSA-N
Formula: C23H28O4
SMILES: CC=Cc1cc(CC)c2c(c1)C(C)C(c1cc(OC)c(OC)c(OC)c1)O2
Mol. weight [g/mol]: 368.47

Physical Properties

Property code	Value	Unit	Source
gf	41.96	kJ/mol	Joback Method
hf	-472.79	kJ/mol	Joback Method
hfus	52.02	kJ/mol	Joback Method
hvap	86.62	kJ/mol	Joback Method
log10ws	-6.73		Crippen Method
logp	5.545		Crippen Method
mcvol	295.730	ml/mol	McGowan Method
pc	1308.01	kPa	Joback Method
rinpol	2770.00		NIST Webbook
rinpol	2770.00		NIST Webbook
tb	909.32	K	Joback Method
tc	1133.72	K	Joback Method
tf	578.81	K	Joback Method
vc	1.119	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	943.50	J/mol×K	909.32	Joback Method
cpg	1013.49	J/mol×K	1096.32	Joback Method
cpg	1002.03	J/mol×K	1058.92	Joback Method
cpg	989.34	J/mol×K	1021.52	Joback Method
cpg	975.37	J/mol×K	984.12	Joback Method
cpg	960.11	J/mol×K	946.72	Joback Method
cpg	1023.75	J/mol×K	1133.72	Joback Method
dvisc	0.0001046	Pa×s	909.32	Joback Method

dvisc	0.0001208	Pa×s	854.24	Joback Method
dvisc	0.0001425	Pa×s	799.15	Joback Method
dvisc	0.0001721	Pa×s	744.07	Joback Method
dvisc	0.0002143	Pa×s	688.98	Joback Method
dvisc	0.0002773	Pa×s	633.90	Joback Method
dvisc	0.0003767	Pa×s	578.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R294454&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

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