ETOXAZOLE

Other names: Oxazole, 2-(2,6-difluorophenyl)-4-[4-(1,1-dimethylethyl)-2-ethoxyphenyl]-4,5-dihydro-
2-(2,6-difluorophenyl)-4-[4-(1,1-dimethylethyl)-2-ethoxyphenyl]-4,5-dihydrooxazole

Inchi: InChI=1S/C21H23F2NO2/c1-5-25-18-11-13(21(2,3)4)9-10-14(18)17-12-26-20(24-17)19-1

InchiKey: IXSZQYVWNJNRAL-UHFFFAOYSA-N

Formula: C21H23F2NO2

SMILES: CCOc1cc(C(C)(C)C)ccc1C1COC(c2c(F)cccc2F)=N1

Mol. weight [g/mol]: 359.41

CAS: 153233-91-1

Physical Properties

Property code	Value	Unit	Source
gf	-92.00	kJ/mol	Joback Method
hf	-537.02	kJ/mol	Joback Method
hfus	44.49	kJ/mol	Joback Method
hvap	80.95	kJ/mol	Joback Method
log10ws	-6.02		Crippen Method
logp	5.179		Crippen Method
mcvol	269.330	ml/mol	McGowan Method
pc	1565.99	kPa	Joback Method
rinpol	2489.00		NIST Webbook
tb	870.96	K	Joback Method
tc	1106.23	K	Joback Method
tf	577.47	K	Joback Method
vc	1.036	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	862.87	J/mol×K	870.96	Joback Method
cpg	879.18	J/mol×K	910.17	Joback Method
cpg	893.92	J/mol×K	949.38	Joback Method
cpg	907.17	J/mol×K	988.59	Joback Method
cpg	918.98	J/mol×K	1027.80	Joback Method
cpg	929.40	J/mol×K	1067.02	Joback Method

cpg	938.51	J/mol×K	1106.23	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=C153233911&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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