Ethofumesate

Other names: (.+/-.)-2-Ethoxy-2,3-dihydro-3,3-dimethyl-5-benzofuranol methanesulfonate
(.+/-.)-2-Ethoxy-2,3-dihydro-3,3-dimethyl-5-benzofuranylmethanesulfonate
(dl)-2-ethoxy-2,3-dihydro-3,3-dimethyl-5-benzofuranylmethanesulfonate
2-Ethoxy-3,3-dimethyl-2,3-dihydro-1-benzofuran-5-yl methanesulfonate
5-Benzofuranol, 2-Ethoxy-2,3-dihydro-3,3-dimethyl-, methanesulfonate
5-Benzofuranol, 2-ethoxy-2,3-dihydro-3,3-dimethyl-, methanesulfonate, (.+/-.)-
CR 14658
NC 8438
Norton
Nortran
Nortranese
Nortron
Nortron (new)
Prograss
Tramat

Inchi: InChI=1S/C13H18O5S/c1-5-16-12-13(2,3)10-8-9(18-19(4,14)15)6-7-11(10)17-12/h6-8,12

InchiKey: IRCMYGHHKLLGHV-UHFFFAOYSA-N

Formula: C13H18O5S

SMILES: CCOC1Oc2ccc(OS(C)(=O)=O)cc2C1(C)C

Mol. weight [g/mol]: 286.34

CAS: 26225-79-6

Physical Properties

Property code	Value	Unit	Source
gf	-565.38	kJ/mol	Joback Method
hf	-880.15	kJ/mol	Joback Method
hfus	37.33	kJ/mol	Joback Method
hvap	74.55	kJ/mol	Joback Method
log10ws	-3.42		Aqueous Solubility Prediction Method
log10ws	-3.42		Estimated Solubility Method
logp	2.058		Crippen Method
mcvol	205.110	ml/mol	McGowan Method
pc	2738.28	kPa	Joback Method
rinpol	1910.00		NIST Webbook
rinpol	1951.00		NIST Webbook

rinpol	1953.00		NIST Webbook
rinpol	1924.00		NIST Webbook
tb	655.36	K	Joback Method
tc	862.89	K	Joback Method
tf	345.62 ± 0.20	K	NIST Webbook
vc	0.792	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	552.27	J/mol×K	655.36	Joback Method
cpg	568.33	J/mol×K	689.95	Joback Method
cpg	583.58	J/mol×K	724.54	Joback Method
cpg	598.09	J/mol×K	759.13	Joback Method
cpg	611.93	J/mol×K	793.71	Joback Method
cpg	625.18	J/mol×K	828.30	Joback Method
cpg	637.92	J/mol×K	862.89	Joback Method
hfust	26.25	kJ/mol	344.10	NIST Webbook

Sources

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C26225796&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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
hfust: Enthalpy of fusion at a given temperature

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