Etofenprox

Other names:	Benzene, 1-[[2-(4-ethoxyphenyl)-2-methylpropoxy]methyl]-3-phenoxy- Ethofenprox «alpha»-[(p-Ethoxy-«beta»,«beta»-dimethylphenethyl)oxy]-m-phenoxytoluene Â«alphaÂ»-[(p-Ethoxy-Â«betaÂ»,Â«betaÂ»-dimethylphenethyl)oxy]-m-phenoxytoluene
Inchi:	InChI=1S/C25H28O3/c1-4-27-22-15-13-21(14-16-22)25(2,3)19-26-18-20-9-8-12-24(17-2
InchiKey:	YREQHYQNNWYQCJ-UHFFFAOYSA-N
Formula:	C25H28O3
SMILES:	CCOc1ccc(C(C)(C)COCc2cccc(Oc3ccccc3)c2)cc1
Mol. weight [g/mol]:	376.49
CAS:	80844-07-1

Physical Properties

Property code	Value	Unit	Source
gf	165.43	kJ/mol	Joback Method
hf	-278.09	kJ/mol	Joback Method
hfus	38.00	kJ/mol	Joback Method
hvap	85.33	kJ/mol	Joback Method
log10ws	-8.60		Estimated Solubility Method
log10ws	-8.60		Aqueous Solubility Prediction Method
logp	6.372		Crippen Method
mcvol	309.440	ml/mol	McGowan Method
pc	1385.05	kPa	Joback Method
rinpol	2870.00		NIST Webbook
rinpol	2887.10		NIST Webbook
rinpol	2826.00		NIST Webbook
rinpol	2826.00		NIST Webbook
rinpol	2870.00		NIST Webbook
rinpol	2880.00		NIST Webbook
tb	925.43	K	Joback Method
tc	1164.34	K	Joback Method
tf	309.65	K	Aqueous Solubility Prediction Method
vc	1.155	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	975.46	J/mol×K	925.43	Joback Method
cpg	991.61	J/mol×K	965.25	Joback Method
cpg	1006.18	J/mol×K	1005.07	Joback Method
cpg	1019.27	J/mol×K	1044.88	Joback Method
cpg	1030.95	J/mol×K	1084.70	Joback Method
cpg	1041.31	J/mol×K	1124.52	Joback Method
cpg	1050.43	J/mol×K	1164.34	Joback Method
dvisc	0.0002154	Pa×s	544.92	Joback Method
dvisc	0.0001152	Pa×s	608.34	Joback Method
dvisc	0.0000694	Pa×s	671.76	Joback Method
dvisc	0.0000456	Pa×s	735.18	Joback Method
dvisc	0.0000320	Pa×s	798.59	Joback Method
dvisc	0.0000237	Pa×s	862.01	Joback Method
dvisc	0.0000183	Pa×s	925.43	Joback Method

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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=C80844071&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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