Flutolanil

Other names:	Benzamide, N-(3-(1-methylethoxy)phenyl)-2-(trifluoromethyl)- Moncut NNF-136 flutoluanil
Inchi:	InChI=1S/C17H16F3NO2/c1-11(2)23-13-7-5-6-12(10-13)21-16(22)14-8-3-4-9-15(14)17(1
InchiKey:	PTCGDEVVHUXTMP-UHFFFAOYSA-N
Formula:	C17H16F3NO2
SMILES:	CC(C)Oc1cccc(NC(=O)c2ccccc2C(F)(F)F)c1
Mol. weight [g/mol]:	323.31
CAS:	66332-96-5

Physical Properties

Property code	Value	Unit	Source
gf	-430.74	kJ/mol	Joback Method
hf	-737.78	kJ/mol	Joback Method
hfus	33.28	kJ/mol	Joback Method
hvap	70.77	kJ/mol	Joback Method
log10ws	-5.62		Crippen Method
logp	4.745		Crippen Method
mcvol	225.600	ml/mol	McGowan Method
pc	1945.79	kPa	Joback Method
tb	772.28	K	Joback Method
tc	989.59	K	Joback Method
tf	473.24	K	Joback Method
vc	0.868	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	650.55	J/mol×K	772.28	Joback Method
cpg	664.41	J/mol×K	808.50	Joback Method
cpg	677.17	J/mol×K	844.72	Joback Method
cpg	688.88	J/mol×K	880.94	Joback Method
cpg	699.63	J/mol×K	917.16	Joback Method

cpg	709.45	J/mol×K	953.37	Joback Method
cpg	718.44	J/mol×K	989.59	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=C66332965&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume