Benzamide, 2,4,5-trifluoro-3-methoxy-N-(2,4,5-trifluoro-3-meth

Inchi: InChI=1S/C23H23F6NO4/c1-5-6-7-8-11(2)30(22(31)12-9-14(24)18(28)20(33-3)16(12)26)

InchiKey: JDZUUWCNYLFYRB-UHFFFAOYSA-N

Formula: C23H23F6NO4

SMILES: CCCCCC(C)N(C(=O)c1cc(F)c(F)c(OC)c1F)C(=O)c1cc(F)c(F)c(OC)c1F

Mol. weight [g/mol]: 491.42

Physical Properties

Property code	Value	Unit	Source
gf	-1237.80	kJ/mol	Joback Method
hf	-1740.76	kJ/mol	Joback Method
hfus	63.85	kJ/mol	Joback Method
hvap	91.70	kJ/mol	Joback Method
log10ws	-8.44		Crippen Method
logp	5.790		Crippen Method
mcvol	322.890	ml/mol	McGowan Method
pc	1070.76	kPa	Joback Method
rinpol	2412.00		NIST Webbook
rinpol	2412.00		NIST Webbook
tb	979.04	K	Joback Method
tc	1199.12	K	Joback Method
tf	667.30	K	Joback Method
vc	1.276	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1033.46	J/mol×K	979.04	Joback Method
cpg	1045.60	J/mol×K	1015.72	Joback Method
cpg	1056.30	J/mol×K	1052.40	Joback Method
cpg	1065.58	J/mol×K	1089.08	Joback Method
cpg	1073.45	J/mol×K	1125.76	Joback Method
cpg	1079.94	J/mol×K	1162.44	Joback Method
cpg	1085.06	J/mol×K	1199.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407660&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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