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

Inchi: InChI=1S/C23H23F6NO4/c1-4-5-6-7-8-9-30(22(31)12-10-14(24)18(28)20(33-2)16(12)26)

InchiKey: CDHIQRKDTWUZJX-UHFFFAOYSA-N

Formula: C23H23F6NO4

SMILES: CCCCCCCN(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	-1235.36	kJ/mol	Joback Method
hf	-1735.48	kJ/mol	Joback Method
hfus	67.37	kJ/mol	Joback Method
hvap	92.09	kJ/mol	Joback Method
log10ws	-8.32		Crippen Method
logp	5.791		Crippen Method
mcvol	322.890	ml/mol	McGowan Method
pc	1065.18	kPa	Joback Method
rinpol	2519.00		NIST Webbook
rinpol	2519.00		NIST Webbook
tb	979.48	K	Joback Method
tc	1200.13	K	Joback Method
tf	682.30	K	Joback Method
vc	1.282	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1033.04	J/mol×K	979.48	Joback Method
cpg	1045.26	J/mol×K	1016.25	Joback Method
cpg	1056.05	J/mol×K	1053.03	Joback Method
cpg	1065.43	J/mol×K	1089.80	Joback Method
cpg	1073.40	J/mol×K	1126.58	Joback Method
cpg	1080.00	J/mol×K	1163.35	Joback Method
cpg	1085.24	J/mol×K	1200.13	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=U407663&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