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

Inchi: InChI=1S/C22H21F6NO4/c1-4-5-6-7-8-29(21(30)11-9-13(23)17(27)19(32-2)15(11)25)22(

InchiKey: VGSOKFCQIRBMIH-UHFFFAOYSA-N

Formula: C22H21F6NO4

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

Mol. weight [g/mol]: 477.40

Physical Properties

Property code	Value	Unit	Source
gf	-1243.78	kJ/mol	Joback Method
hf	-1714.84	kJ/mol	Joback Method
hfus	64.78	kJ/mol	Joback Method
hvap	89.87	kJ/mol	Joback Method
log10ws	-7.90		Crippen Method
logp	5.401		Crippen Method
mcvol	308.800	ml/mol	McGowan Method
pc	1135.20	kPa	Joback Method
rinpol	2421.00		NIST Webbook
tb	956.60	K	Joback Method
tc	1171.21	K	Joback Method
tf	671.03	K	Joback Method
vc	1.226	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	974.10	J/mol×K	956.60	Joback Method
cpg	986.06	J/mol×K	992.37	Joback Method
cpg	996.71	J/mol×K	1028.14	Joback Method
cpg	1006.05	J/mol×K	1063.91	Joback Method
cpg	1014.10	J/mol×K	1099.68	Joback Method
cpg	1020.88	J/mol×K	1135.44	Joback Method
cpg	1026.38	J/mol×K	1171.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407661&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

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