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

Inchi: InChI=1S/C28H33F6NO4/c1-4-5-6-7-8-9-10-11-12-13-14-35(27(36)17-15-19(29)23(33)25

InchiKey: VPLPBRHMVAPPBK-UHFFFAOYSA-N

Formula: C28H33F6NO4

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

Mol. weight [g/mol]: 561.56

Physical Properties

Property code	Value	Unit	Source
gf	-1193.26	kJ/mol	Joback Method
hf	-1838.68	kJ/mol	Joback Method
hfus	80.32	kJ/mol	Joback Method
hvap	103.22	kJ/mol	Joback Method
log10ws	-10.42		Crippen Method
logp	7.742		Crippen Method
mcvol	393.340	ml/mol	McGowan Method
pc	796.18	kPa	Joback Method
rinpol	3018.00		NIST Webbook
rinpol	3018.00		NIST Webbook
tb	1093.88	K	Joback Method
tc	1363.33	K	Joback Method
tf	738.65	K	Joback Method
vc	1.562	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1333.84	J/mol×K	1093.88	Joback Method
cpg	1347.26	J/mol×K	1138.79	Joback Method
cpg	1358.35	J/mol×K	1183.70	Joback Method
cpg	1367.18	J/mol×K	1228.61	Joback Method
cpg	1373.80	J/mol×K	1273.51	Joback Method
cpg	1378.29	J/mol×K	1318.42	Joback Method
cpg	1380.71	J/mol×K	1363.33	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=U407668&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