

Benzamide, 2,4,5-trifluoro-3-methoxy-N-(2,4,5-trifluoro-3-methoxyphenyl)

Inchi: InChI=1S/C27H31F6NO4/c1-4-5-6-7-8-9-10-11-12-13-34(26(35)16-14-18(28)22(32)24(33)27)/n27
InchiKey: YLMUNOXRRWPBLS-UHFFFAOYSA-N
Formula: C27H31F6NO4
SMILES: CCCCCCCCCCN(C(=O)c1cc(F)c(F)c(OC)c1F)C(=O)c1cc(F)c(F)c(OC)c1F
Mol. weight [g/mol]: 547.53

Physical Properties

Property code	Value	Unit	Source
gf	-1201.68	kJ/mol	Joback Method
hf	-1818.04	kJ/mol	Joback Method
hfus	77.73	kJ/mol	Joback Method
hvap	101.00	kJ/mol	Joback Method
log10ws	-10.00		Crippen Method
logp	7.352		Crippen Method
mvol	379.250	ml/mol	McGowan Method
pc	841.13	kPa	Joback Method
rinpol	2916.00		NIST Webbook
rinpol	2916.00		NIST Webbook
tb	1071.00	K	Joback Method
tc	1327.89	K	Joback Method
tf	727.38	K	Joback Method
vc	1.506	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1273.03	J/molxK	1071.00	Joback Method
cpg	1286.23	J/molxK	1113.81	Joback Method
cpg	1297.33	J/molxK	1156.63	Joback Method
cpg	1306.39	J/molxK	1199.44	Joback Method
cpg	1313.45	J/molxK	1242.26	Joback Method
cpg	1318.57	J/molxK	1285.07	Joback Method
cpg	1321.79	J/molxK	1327.89	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=U407667&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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