

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

Inchi: InChI=1S/C24H25F6NO4/c1-5-7-8-12(6-2)11-31(23(32)13-9-15(25)19(29)21(34-3)17(13)-14)22-4
InchiKey: APGXXPORVCDESS-UHFFFAOYSA-N
Formula: C24H25F6NO4
SMILES: CCCCC(C)CN(C(=O)c1cc(F)c(F)c(OC)c1F)C(=O)c1cc(F)c(F)c(OC)c1F
Mol. weight [g/mol]: 505.45

Physical Properties

Property code	Value	Unit	Source
gf	-1229.38	kJ/mol	Joback Method
hf	-1761.40	kJ/mol	Joback Method
hfus	66.44	kJ/mol	Joback Method
hvap	93.93	kJ/mol	Joback Method
log10ws	-8.50		Crippen Method
logp	6.037		Crippen Method
mcvol	336.980	ml/mol	McGowan Method
pc	1006.53	kPa	Joback Method
rinpol	2502.00		NIST Webbook
rinpol	2502.00		NIST Webbook
tb	1001.92	K	Joback Method
tc	1228.72	K	Joback Method
tf	678.57	K	Joback Method
vc	1.331	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1092.83	J/molxK	1001.92	Joback Method
cpg	1105.19	J/molxK	1039.72	Joback Method
cpg	1115.99	J/molxK	1077.52	Joback Method
cpg	1125.24	J/molxK	1115.32	Joback Method
cpg	1132.98	J/molxK	1153.12	Joback Method
cpg	1139.21	J/molxK	1190.92	Joback Method
cpg	1143.97	J/molxK	1228.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407662&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
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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