

Benzamide, 3-fluoro-4-trifluoromethyl-N-(3-fluoro-4-trifluoromethylphenyl)

Inchi: InChI=1S/C24H23F8NO2/c1-3-5-6-14(4-2)13-33(21(34)15-7-9-17(19(25)11-15)23(27,28)12)20-22
InchiKey: SZZQBTSBOSQZQJ-UHFFFAOYSA-N
Formula: C24H23F8NO2
SMILES: CCCCC(CC)CN(C(=O)c1ccc(C(F)(F)F)c(F)c1)C(=O)c1ccc(C(F)(F)F)c(F)c1
Mol. weight [g/mol]: 509.43

Physical Properties

Property code	Value	Unit	Source
gf	-1364.80	kJ/mol	Joback Method
hf	-1860.80	kJ/mol	Joback Method
hfus	56.95	kJ/mol	Joback Method
hvap	82.24	kJ/mol	Joback Method
log10ws	-9.14		Crippen Method
logp	7.501		Crippen Method
mcvol	328.780	ml/mol	McGowan Method
pc	1033.90	kPa	Joback Method
rinpol	2138.00		NIST Webbook
rinpol	2138.00		NIST Webbook
tb	929.24	K	Joback Method
tc	1137.90	K	Joback Method
tf	590.05	K	Joback Method
vc	1.310	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1057.90	J/molxK	929.24	Joback Method
cpg	1071.40	J/molxK	964.02	Joback Method
cpg	1083.98	J/molxK	998.79	Joback Method
cpg	1095.77	J/molxK	1033.57	Joback Method
cpg	1106.86	J/molxK	1068.34	Joback Method
cpg	1117.37	J/molxK	1103.12	Joback Method
cpg	1127.40	J/molxK	1137.90	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=U407909&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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