

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

Inchi:	InChI=1S/C20H15F8NO2/c1-10(2)9-29(17(30)11-3-5-13(15(21)7-11)19(23,24)25)18(31)
InchiKey:	MGIJVFWSDJQKTA-UHFFFAOYSA-N
Formula:	C20H15F8NO2
SMILES:	CC(C)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]:	453.33

Physical Properties

Property code	Value	Unit	Source
gf	-1398.48	kJ/mol	Joback Method
hf	-1778.24	kJ/mol	Joback Method
hfus	46.59	kJ/mol	Joback Method
hvap	73.33	kJ/mol	Joback Method
log10ws	-7.47		Crippen Method
logp	5.941		Crippen Method
mvol	272.420	ml/mol	McGowan Method
pc	1345.70	kPa	Joback Method
rinpol	1833.00		NIST Webbook
rinpol	1833.00		NIST Webbook
tb	837.72	K	Joback Method
tc	1035.62	K	Joback Method
tf	544.97	K	Joback Method
vc	1.085	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	827.26	J/molxK	837.72	Joback Method
cpg	839.15	J/molxK	870.70	Joback Method
cpg	850.16	J/molxK	903.69	Joback Method
cpg	860.37	J/molxK	936.67	Joback Method
cpg	869.86	J/molxK	969.66	Joback Method
cpg	878.73	J/molxK	1002.64	Joback Method
cpg	887.05	J/molxK	1035.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407904&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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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