

Benzamide, 3-fluoro-5-trifluoromethyl-N-(3-fluoro-5-trifluoromethyl)

Inchi:	InChI=1S/C19H13F8NO2/c1-2-5-28(16(29)10-6-11(18(22,23)24)8-13(21)7-10)17(30)14-9
InchiKey:	BJCXHNAUCKTPPF-UHFFFAOYSA-N
Formula:	C19H13F8NO2
SMILES:	CCCN(C(=O)c1cc(F)cc(C(F)(F)F)c1)C(=O)c1cc(F)ccc1C(F)(F)F
Mol. weight [g/mol]:	439.30

Physical Properties

Property code	Value	Unit	Source
gf	-1404.46	kJ/mol	Joback Method
hf	-1752.32	kJ/mol	Joback Method
hfus	47.52	kJ/mol	Joback Method
hvap	71.49	kJ/mol	Joback Method
log10ws	-7.29		Crippen Method
logp	5.695		Crippen Method
mcvol	258.330	ml/mol	McGowan Method
pc	1436.98	kPa	Joback Method
rinpol	1648.00		NIST Webbook
rinpol	1648.00		NIST Webbook
tb	815.28	K	Joback Method
tc	1010.63	K	Joback Method
tf	548.70	K	Joback Method
vc	1.036	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	771.05	J/molxK	815.28	Joback Method
cpg	782.49	J/molxK	847.84	Joback Method
cpg	793.08	J/molxK	880.40	Joback Method
cpg	802.89	J/molxK	912.95	Joback Method
cpg	812.01	J/molxK	945.51	Joback Method
cpg	820.50	J/molxK	978.07	Joback Method
cpg	828.45	J/molxK	1010.63	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U407868&Units=SI

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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