

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

Inchi: InChI=1S/C21H17F8NO2/c1-11(2)5-6-30(18(31)12-7-13(20(24,25)26)9-15(23)8-12)19(32)3
InchiKey: ZHVXUUHKRVYEHB-UHFFFAOYSA-N
Formula: C21H17F8NO2
SMILES: CC(C)CCN(C(=O)c1cc(F)cc(C(F)(F)F)c1)C(=O)c1cc(F)ccc1C(F)(F)F
Mol. weight [g/mol]: 467.35

Physical Properties

Property code	Value	Unit	Source
gf	-1390.06	kJ/mol	Joback Method
hf	-1798.88	kJ/mol	Joback Method
hfus	49.18	kJ/mol	Joback Method
hvap	75.56	kJ/mol	Joback Method
log10ws	-7.89		Crippen Method
logp	6.331		Crippen Method
mvol	286.510	ml/mol	McGowan Method
pc	1255.70	kPa	Joback Method
rinpol	1765.00		NIST Webbook
rinpol	1765.00		NIST Webbook
tb	860.60	K	Joback Method
tc	1059.97	K	Joback Method
tf	556.24	K	Joback Method
vc	1.141	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	883.75	J/molxK	860.60	Joback Method
cpg	895.99	J/molxK	893.83	Joback Method
cpg	907.36	J/molxK	927.06	Joback Method
cpg	917.92	J/molxK	960.29	Joback Method
cpg	927.78	J/molxK	993.52	Joback Method
cpg	937.02	J/molxK	1026.75	Joback Method
cpg	945.73	J/molxK	1059.97	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=U407871&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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