

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

Inchi: InChI=1S/C22H19F8NO2/c1-2-3-4-5-10-31(19(32)13-6-8-15(17(23)11-13)21(25,26)27)20
InchiKey: IMNMDUBDZYUNLH-UHFFFAOYSA-N
Formula: C22H19F8NO2
SMILES: CCCCCN(C(=O)c1ccc(C(F)(F)F)c(F)c1)C(=O)c1ccc(C(F)(F)F)c(F)c1
Mol. weight [g/mol]: 481.38

Physical Properties

Property code	Value	Unit	Source
gf	-1379.20	kJ/mol	Joback Method
hf	-1814.24	kJ/mol	Joback Method
hfus	55.29	kJ/mol	Joback Method
hvap	78.17	kJ/mol	Joback Method
log10ws	-8.55		Crippen Method
logp	6.865		Crippen Method
mcvol	300.600	ml/mol	McGowan Method
pc	1168.02	kPa	Joback Method
rinpol	2066.00		NIST Webbook
rinpol	2066.00		NIST Webbook
tb	883.92	K	Joback Method
tc	1084.71	K	Joback Method
tf	582.51	K	Joback Method
vc	1.204	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	940.51	J/molxK	883.92	Joback Method
cpg	953.11	J/molxK	917.39	Joback Method
cpg	964.84	J/molxK	950.85	Joback Method
cpg	975.79	J/molxK	984.32	Joback Method
cpg	986.06	J/molxK	1017.78	Joback Method
cpg	995.73	J/molxK	1051.25	Joback Method
cpg	1004.90	J/molxK	1084.71	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407908&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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