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

Inchi: InChI=1S/C22H19F8NO2/c1-2-3-4-5-8-31(19(32)13-9-14(21(25,26)27)11-16(24)10-13)20

InchiKey: XJSBHFOVSOXVAG-UHFFFAOYSA-N

Formula: C22H19F8NO2

SMILES: CCCCCCN(C(=O)c1cc(F)cc(C(F)(F)F)c1)C(=O)c1cc(F)ccc1C(F)(F)F

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	1897.00		NIST Webbook
rinpol	1897.00		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/mol×K	883.92	Joback Method
cpg	953.11	J/mol×K	917.39	Joback Method
cpg	964.84	J/mol×K	950.85	Joback Method
cpg	975.79	J/mol×K	984.32	Joback Method
cpg	986.06	J/mol×K	1017.78	Joback Method
cpg	995.73	J/mol×K	1051.25	Joback Method
cpg	1004.90	J/mol×K	1084.71	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407874&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
hvap:	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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume