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

Inchi: InChI=1S/C23H21F8NO2/c1-2-3-4-5-6-9-32(20(33)14-10-15(22(26,27)28)12-17(25)11-14

InchiKey: CRWPQZFOYBDMBK-UHFFFAOYSA-N

Formula: C23H21F8NO2

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

Mol. weight [g/mol]: 495.41

Physical Properties

Property code	Value	Unit	Source
gf	-1370.78	kJ/mol	Joback Method
hf	-1834.88	kJ/mol	Joback Method
hfus	57.88	kJ/mol	Joback Method
hvap	80.40	kJ/mol	Joback Method
log10ws	-8.96		Crippen Method
logp	7.255		Crippen Method
mcvol	314.690	ml/mol	McGowan Method
pc	1094.99	kPa	Joback Method
rinpol	1988.00		NIST Webbook
rinpol	1988.00		NIST Webbook
tb	906.80	K	Joback Method
tc	1111.02	K	Joback Method
tf	593.78	K	Joback Method
vc	1.260	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	998.60	J/mol×K	906.80	Joback Method
cpg	1011.65	J/mol×K	940.84	Joback Method
cpg	1023.81	J/mol×K	974.87	Joback Method
cpg	1035.18	J/mol×K	1008.91	Joback Method
cpg	1045.88	J/mol×K	1042.95	Joback Method
cpg	1055.99	J/mol×K	1076.98	Joback Method
cpg	1065.62	J/mol×K	1111.02	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407876&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
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

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