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

Inchi: InChI=1S/C25H25F8NO2/c1-2-3-4-5-6-7-8-11-34(22(35)16-12-17(24(28,29)30)14-19(27)

InchiKey: YTPPJHGOCUOXCB-UHFFFAOYSA-N

Formula: C25H25F8NO2

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

Mol. weight [g/mol]: 523.46

Physical Properties

Property code	Value	Unit	Source
gf	-1353.94	kJ/mol	Joback Method
hf	-1876.16	kJ/mol	Joback Method
hfus	63.06	kJ/mol	Joback Method
hvap	84.85	kJ/mol	Joback Method
log10ws	-9.80		Crippen Method
logp	8.036		Crippen Method
mcvol	342.870	ml/mol	McGowan Method
pc	968.07	kPa	Joback Method
rinpol	2176.00		NIST Webbook
rinpol	2176.00		NIST Webbook
tb	952.56	K	Joback Method
tc	1166.44	K	Joback Method
tf	616.32	K	Joback Method
vc	1.371	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1116.95	J/mol×K	952.56	Joback Method
cpg	1131.01	J/mol×K	988.21	Joback Method
cpg	1144.16	J/mol×K	1023.85	Joback Method
cpg	1156.52	J/mol×K	1059.50	Joback Method
cpg	1168.21	J/mol×K	1095.15	Joback Method
cpg	1179.35	J/mol×K	1130.79	Joback Method
cpg	1190.06	J/mol×K	1166.44	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407878&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