Benzamide, 2-trifluoromethyl-5-fluoro-N-(2-trifluoromethyl-5-fl

Inchi: InChI=1S/C20H15F8NO2/c1-10(2)9-29(17(30)13-7-11(21)3-5-15(13)19(23,24)25)18(31)1

InchiKey: WIPYZERMAHCIGC-UHFFFAOYSA-N

Formula: C20H15F8NO2

SMILES: CC(C)CN(C(=O)c1cc(F)ccc1C(F)(F)F)C(=O)c1cc(F)ccc1C(F)(F)F

Mol. weight [g/mol]: 453.33

Physical Properties

Property code	Value	Unit	Source
gf	-1398.48	kJ/mol	Joback Method
hf	-1778.24	kJ/mol	Joback Method
hfus	46.59	kJ/mol	Joback Method
hvap	73.33	kJ/mol	Joback Method
log10ws	-7.47		Crippen Method
logp	5.941		Crippen Method
mcvol	272.420	ml/mol	McGowan Method
pc	1345.70	kPa	Joback Method
rinpol	1884.00		NIST Webbook
rinpol	1884.00		NIST Webbook
tb	837.72	K	Joback Method
tc	1035.62	K	Joback Method
tf	544.97	K	Joback Method
vc	1.085	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	827.26	J/mol×K	837.72	Joback Method
cpg	839.15	J/mol×K	870.70	Joback Method
cpg	850.16	J/mol×K	903.69	Joback Method
cpg	860.37	J/mol×K	936.67	Joback Method
cpg	869.86	J/mol×K	969.66	Joback Method
cpg	878.73	J/mol×K	1002.64	Joback Method
cpg	887.05	J/mol×K	1035.62	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407694&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
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
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