Benzamide, 3-trifluoromethyl-2-fluoro-N-(3-trifluoromethyl-2-fl

Inchi: InChI=1S/C20H15F8NO2/c1-2-3-10-29(17(30)11-6-4-8-13(15(11)21)19(23,24)25)18(31)1

InchiKey: HHQPLRFAYZHQBL-UHFFFAOYSA-N

Formula: C20H15F8NO2

SMILES: CCCCN(C(=O)c1cccc(C(F)(F)F)c1F)C(=O)c1cccc(C(F)(F)F)c1F

Mol. weight [g/mol]: 453.33

Physical Properties

Property code	Value	Unit	Source
gf	-1396.04	kJ/mol	Joback Method
hf	-1772.96	kJ/mol	Joback Method
hfus	50.11	kJ/mol	Joback Method
hvap	73.72	kJ/mol	Joback Method
log10ws	-7.71		Crippen Method
logp	6.085		Crippen Method
mcvol	272.420	ml/mol	McGowan Method
pc	1337.84	kPa	Joback Method
rinpol	1948.00		NIST Webbook
rinpol	1948.00		NIST Webbook
tb	838.16	K	Joback Method
tc	1034.58	K	Joback Method
tf	559.97	K	Joback Method
vc	1.091	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	826.69	J/mol×K	838.16	Joback Method
cpg	838.50	J/mol×K	870.90	Joback Method
cpg	849.45	J/mol×K	903.63	Joback Method
cpg	859.63	J/mol×K	936.37	Joback Method
cpg	869.12	J/mol×K	969.10	Joback Method
cpg	877.99	J/mol×K	1001.84	Joback Method
cpg	886.33	J/mol×K	1034.58	Joback Method

Sources

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=U407720&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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