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

Inchi: InChI=1S/C19H13F8NO2/c1-2-9-28(16(29)10-5-3-7-12(14(10)20)18(22,23)24)17(30)11-6

InchiKey: KYBQGARLXBDTQQ-UHFFFAOYSA-N

Formula: C19H13F8NO2

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

Mol. weight [g/mol]: 439.30

Physical Properties

Property code	Value	Unit	Source
gf	-1404.46	kJ/mol	Joback Method
hf	-1752.32	kJ/mol	Joback Method
hfus	47.52	kJ/mol	Joback Method
hvap	71.49	kJ/mol	Joback Method
log10ws	-7.29		Crippen Method
logp	5.695		Crippen Method
mcvol	258.330	ml/mol	McGowan Method
pc	1436.98	kPa	Joback Method
rinpol	1862.00		NIST Webbook
rinpol	1862.00		NIST Webbook
tb	815.28	K	Joback Method
tc	1010.63	K	Joback Method
tf	548.70	K	Joback Method
vc	1.036	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	771.05	J/mol×K	815.28	Joback Method
cpg	782.49	J/mol×K	847.84	Joback Method
cpg	793.08	J/mol×K	880.40	Joback Method
cpg	802.89	J/mol×K	912.95	Joback Method
cpg	812.01	J/mol×K	945.51	Joback Method
cpg	820.50	J/mol×K	978.07	Joback Method
cpg	828.45	J/mol×K	1010.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407718&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