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

Inchi: InChI=1S/C24H23F8NO2/c1-3-5-8-14(4-2)13-33(21(34)15-9-6-11-17(19(15)25)23(27,28)

InchiKey: OXDWOJXQHHYJCU-UHFFFAOYSA-N

Formula: C24H23F8NO2

SMILES: CCCCC(CC)CN(C(=O)c1cccc(C(F)(F)F)c1F)C(=O)c1cccc(C(F)(F)F)c1F

Mol. weight [g/mol]: 509.43

Physical Properties

Property code	Value	Unit	Source
gf	-1364.80	kJ/mol	Joback Method
hf	-1860.80	kJ/mol	Joback Method
hfus	56.95	kJ/mol	Joback Method
hvap	82.24	kJ/mol	Joback Method
log10ws	-9.14		Crippen Method
logp	7.501		Crippen Method
mcvol	328.780	ml/mol	McGowan Method
pc	1033.90	kPa	Joback Method
rinpol	2223.00		NIST Webbook
rinpol	2223.00		NIST Webbook
tb	929.24	K	Joback Method
tc	1137.90	K	Joback Method
tf	590.05	K	Joback Method
vc	1.310	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1057.90	J/mol×K	929.24	Joback Method
cpg	1071.40	J/mol×K	964.02	Joback Method
cpg	1083.98	J/mol×K	998.79	Joback Method
cpg	1095.77	J/mol×K	1033.57	Joback Method
cpg	1106.86	J/mol×K	1068.34	Joback Method
cpg	1117.37	J/mol×K	1103.12	Joback Method
cpg	1127.40	J/mol×K	1137.90	Joback Method

Sources

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=U407725&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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