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

Inchi: InChI=1S/C17H9F8NO2/c1-26(14(27)8-4-9(16(20,21)22)6-11(19)5-8)15(28)12-7-10(18)2

InchiKey: VUCDSNOVKCJEPZ-UHFFFAOYSA-N

Formula: C17H9F8NO2

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

Mol. weight [g/mol]: 411.25

Physical Properties

Property code	Value	Unit	Source
gf	-1421.30	kJ/mol	Joback Method
hf	-1711.04	kJ/mol	Joback Method
hfus	42.34	kJ/mol	Joback Method
hvap	67.04	kJ/mol	Joback Method
log10ws	-6.45		Crippen Method
logp	4.915		Crippen Method
mcvol	230.150	ml/mol	McGowan Method
pc	1671.43	kPa	Joback Method
rinpol	1576.00		NIST Webbook
rinpol	1576.00		NIST Webbook
tb	769.52	K	Joback Method
tc	964.70	K	Joback Method
tf	526.16	K	Joback Method
vc	0.923	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	662.57	J/mol×K	769.52	Joback Method
cpg	673.28	J/mol×K	802.05	Joback Method
cpg	683.13	J/mol×K	834.58	Joback Method
cpg	692.21	J/mol×K	867.11	Joback Method
cpg	700.58	J/mol×K	899.64	Joback Method
cpg	708.32	J/mol×K	932.17	Joback Method
cpg	715.49	J/mol×K	964.70	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=U407866&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