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

Inchi: InChI=1S/C18H11F8NO2/c1-2-27(15(28)11-7-9(19)3-5-13(11)17(21,22)23)16(29)12-8-10

InchiKey: RKMOSNJWSYZVJI-UHFFFAOYSA-N

Formula: C18H11F8NO2

SMILES: CCN(C(=O)c1cc(F)ccc1C(F)(F)F)C(=O)c1cc(F)ccc1C(F)(F)F

Mol. weight [g/mol]: 425.27

Physical Properties

Property code	Value	Unit	Source
gf	-1412.88	kJ/mol	Joback Method
hf	-1731.68	kJ/mol	Joback Method
hfus	44.93	kJ/mol	Joback Method
hvap	69.27	kJ/mol	Joback Method
log10ws	-6.87		Crippen Method
logp	5.305		Crippen Method
mcvol	244.240	ml/mol	McGowan Method
pc	1547.57	kPa	Joback Method
rinpol	1785.00		NIST Webbook
rinpol	1785.00		NIST Webbook
tb	792.40	K	Joback Method
tc	987.35	K	Joback Method
tf	537.43	K	Joback Method
vc	0.980	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	716.32	J/mol×K	792.40	Joback Method
cpg	727.40	J/mol×K	824.89	Joback Method
cpg	737.63	J/mol×K	857.38	Joback Method
cpg	747.07	J/mol×K	889.88	Joback Method
cpg	755.82	J/mol×K	922.37	Joback Method
cpg	763.94	J/mol×K	954.86	Joback Method
cpg	771.51	J/mol×K	987.35	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407692&Units=SI

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