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

Inchi: InChI=1S/C28H31F8NO2/c1-2-3-4-5-6-7-8-9-10-11-14-37(25(38)19-15-20(27(31,32)33)1

InchiKey: KRURMGWNTKJBID-UHFFFAOYSA-N

Formula: C28H31F8NO2

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

Mol. weight [g/mol]: 565.54

Physical Properties

Property code	Value	Unit	Source
gf	-1328.68	kJ/mol	Joback Method
hf	-1938.08	kJ/mol	Joback Method
hfus	70.83	kJ/mol	Joback Method
hvap	91.53	kJ/mol	Joback Method
log10ws	-11.06		Crippen Method
logp	9.206		Crippen Method
mcvol	385.140	ml/mol	McGowan Method
pc	815.39	kPa	Joback Method
rinpol	2462.00		NIST Webbook
rinpol	2462.00		NIST Webbook
tb	1021.20	K	Joback Method
tc	1257.69	K	Joback Method
tf	650.13	K	Joback Method
vc	1.540	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1299.35	J/mol×K	1021.20	Joback Method
cpg	1315.46	J/mol×K	1060.62	Joback Method
cpg	1330.59	J/mol×K	1100.03	Joback Method
cpg	1344.93	J/mol×K	1139.45	Joback Method
cpg	1358.65	J/mol×K	1178.86	Joback Method
cpg	1371.93	J/mol×K	1218.28	Joback Method
cpg	1384.95	J/mol×K	1257.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407880&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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