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

Inchi: InChI=1S/C26H27F8NO2/c1-2-3-4-5-6-7-8-9-12-35(23(36)17-13-18(25(29,30)31)15-20(2

InchiKey: FSQCDGXXTXNXCF-UHFFFAOYSA-N

Formula: C26H27F8NO2

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

Mol. weight [g/mol]: 537.49

Physical Properties

Property code	Value	Unit	Source
gf	-1345.52	kJ/mol	Joback Method
hf	-1896.80	kJ/mol	Joback Method
hfus	65.65	kJ/mol	Joback Method
hvap	87.08	kJ/mol	Joback Method
log10ws	-10.22		Crippen Method
logp	8.426		Crippen Method
mcvol	356.960	ml/mol	McGowan Method
pc	912.73	kPa	Joback Method
rinpol	2271.00		NIST Webbook
rinpol	2271.00		NIST Webbook
tb	975.44	K	Joback Method
tc	1195.69	K	Joback Method
tf	627.59	K	Joback Method
vc	1.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1177.13	J/mol×K	975.44	Joback Method
cpg	1191.79	J/mol×K	1012.15	Joback Method
cpg	1205.53	J/mol×K	1048.86	Joback Method
cpg	1218.46	J/mol×K	1085.57	Joback Method
cpg	1230.74	J/mol×K	1122.28	Joback Method
cpg	1242.50	J/mol×K	1158.98	Joback Method
cpg	1253.86	J/mol×K	1195.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407879&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