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

Inchi: InChI=1S/C21H17F8NO2/c1-2-3-4-7-30(18(31)12-8-13(20(24,25)26)10-15(23)9-12)19(32

InchiKey: SBOGREQKNKVMRU-UHFFFAOYSA-N

Formula: C21H17F8NO2

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

Mol. weight [g/mol]: 467.35

Physical Properties

Property code	Value	Unit	Source
gf	-1387.62	kJ/mol	Joback Method
hf	-1793.60	kJ/mol	Joback Method
hfus	52.70	kJ/mol	Joback Method
hvap	75.95	kJ/mol	Joback Method
log10ws	-8.13		Crippen Method
logp	6.475		Crippen Method
mcvol	286.510	ml/mol	McGowan Method
pc	1248.61	kPa	Joback Method
rinpol	1805.00		NIST Webbook
rinpol	1805.00		NIST Webbook
tb	861.04	K	Joback Method
tc	1059.25	K	Joback Method
tf	571.24	K	Joback Method
vc	1.147	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	883.19	J/mol×K	861.04	Joback Method
cpg	895.38	J/mol×K	894.08	Joback Method
cpg	906.72	J/mol×K	927.11	Joback Method
cpg	917.27	J/mol×K	960.15	Joback Method
cpg	927.14	J/mol×K	993.18	Joback Method
cpg	936.40	J/mol×K	1026.22	Joback Method
cpg	945.14	J/mol×K	1059.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407872&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