Benzeneamine, 3-isopropyloxy, N-2-trifluoromethylbenzoyl

Inchi: InChI=1S/C18H18F3NO2/c1-12(2)24-14-7-5-6-13(10-14)11-22-17(23)15-8-3-4-9-16(15)1

InchiKey: IGEYRLXBAHPXCP-UHFFFAOYSA-N

Formula: C18H18F3NO2

SMILES: CC(C)Oc1cccc(CNC(=O)c2ccccc2C(F)(F)F)c1

Mol. weight [g/mol]: 337.34

Physical Properties

Property code	Value	Unit	Source
gf	-422.32	kJ/mol	Joback Method
hf	-758.42	kJ/mol	Joback Method
hfus	35.87	kJ/mol	Joback Method
hvap	73.00	kJ/mol	Joback Method
log10ws	-6.10		Crippen Method
logp	4.423		Crippen Method
mcvol	239.690	ml/mol	McGowan Method
pc	1790.91	kPa	Joback Method
rinpol	2185.00		NIST Webbook
rinpol	2185.00		NIST Webbook
tb	795.16	K	Joback Method
tc	1010.04	K	Joback Method
tf	484.51	K	Joback Method
vc	0.923	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	705.65	J/mol×K	795.16	Joback Method
cpg	719.75	J/mol×K	830.97	Joback Method
cpg	732.74	J/mol×K	866.79	Joback Method
cpg	744.69	J/mol×K	902.60	Joback Method
cpg	755.67	J/mol×K	938.41	Joback Method
cpg	765.74	J/mol×K	974.23	Joback Method
cpg	774.97	J/mol×K	1010.04	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=R537538&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