Isopropyl N-(3-trifluoromethylphenyl)carbamate

Other names: isopropyl m-trifluoromethylcarbanilate
Inchi: InChI=1S/C11H12F3NO2/c1-7(2)17-10(16)15-9-5-3-4-8(6-9)11(12,13)14/h3-7H,1-2H3,(H
InchiKey: BXBUGIFDTNEDNS-UHFFFAOYSA-N
Formula: C11H12F3NO2
SMILES: CC(C)OC(=O)Nc1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 247.21
CAS: 370-56-9

Physical Properties

Property code	Value	Unit	Source
gf	-584.04	kJ/mol	Joback Method
hf	-839.00	kJ/mol	Joback Method
hfus	24.09	kJ/mol	Joback Method
hvap	54.48	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	3.662		Crippen Method
mcvol	164.820	ml/mol	McGowan Method
pc	2482.59	kPa	Joback Method
tb	603.34	K	Joback Method
tc	801.03	K	Joback Method
tf	366.68	K	Joback Method
vc	0.639	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	423.99	J/mol×K	603.34	Joback Method
cpg	437.04	J/mol×K	636.29	Joback Method
cpg	449.26	J/mol×K	669.24	Joback Method
cpg	460.67	J/mol×K	702.19	Joback Method
cpg	471.31	J/mol×K	735.14	Joback Method
cpg	481.21	J/mol×K	768.09	Joback Method
cpg	490.41	J/mol×K	801.03	Joback Method

Sources

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=C370569&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume