Benzamide, 3-trifluoromethyl-2-fluoro-N-methyl-

Inchi: InChI=1S/C9H7F4NO/c1-14-8(15)5-3-2-4-6(7(5)10)9(11,12)13/h2-4H,1H3,(H,14,15)
InchiKey: UFGSMQGJSZTAFB-UHFFFAOYSA-N
Formula: C9H7F4NO
SMILES: CNC(=O)c1cccc(C(F)(F)F)c1F
Mol. weight [g/mol]: 221.15

Physical Properties

Property code	Value	Unit	Source
gf	-697.88	kJ/mol	Joback Method
hf	-867.80	kJ/mol	Joback Method
hfus	23.93	kJ/mol	Joback Method
hvap	47.85	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	2.204		Crippen Method
mcvol	132.540	ml/mol	McGowan Method
pc	2871.95	kPa	Joback Method
rinpol	1294.00		NIST Webbook
rinpol	1294.00		NIST Webbook
tb	539.85	K	Joback Method
tc	732.38	K	Joback Method
tf	350.02	K	Joback Method
vc	0.533	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	314.31	J/mol×K	539.85	Joback Method
cpg	325.12	J/mol×K	571.94	Joback Method
cpg	335.21	J/mol×K	604.03	Joback Method
cpg	344.64	J/mol×K	636.12	Joback Method
cpg	353.42	J/mol×K	668.21	Joback Method
cpg	361.59	J/mol×K	700.30	Joback Method
cpg	369.20	J/mol×K	732.38	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=U407697&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume