Benzamide, N-(2-fluorophenyl)-2-trifluoromethyl-

Inchi: InChI=1S/C14H9F4NO/c15-11-7-3-4-8-12(11)19-13(20)9-5-1-2-6-10(9)14(16,17)18/h1-8I

InchiKey: OVMZEPZVFSXHJV-UHFFFAOYSA-N

Formula: C14H9F4NO

SMILES: O=C(Nc1ccccc1F)c1ccccc1C(F)(F)F

Mol. weight [g/mol]: 283.22

Physical Properties

Property code	Value	Unit	Source
gf	-543.37	kJ/mol	Joback Method
hf	-734.47	kJ/mol	Joback Method
hfus	30.92	kJ/mol	Joback Method
hvap	61.25	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	4.097		Crippen Method
mcvol	179.230	ml/mol	McGowan Method
pc	2462.92	kPa	Joback Method
rinpol	1747.00		NIST Webbook
rinpol	1747.00		NIST Webbook
tb	680.93	K	Joback Method
tc	897.52	K	Joback Method
tf	432.79	K	Joback Method
vc	0.706	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	474.24	J/mol×K	680.93	Joback Method
cpg	486.63	J/mol×K	717.03	Joback Method
cpg	498.00	J/mol×K	753.13	Joback Method
cpg	508.43	J/mol×K	789.23	Joback Method
cpg	517.98	J/mol×K	825.33	Joback Method
cpg	526.73	J/mol×K	861.42	Joback Method
cpg	534.75	J/mol×K	897.52	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=U308530&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