Benzamide, 3-fluoro-5-trifluoromethyl-N-isobutyl-

Inchi: InChI=1S/C12H13F4NO/c1-7(2)6-17-11(18)8-3-9(12(14,15)16)5-10(13)4-8/h3-5,7H,6H2,

InchiKey: VVCIPXUQNJUWQC-UHFFFAOYSA-N

Formula: C12H13F4NO

SMILES: CC(C)CNC(=O)c1cc(F)cc(C(F)(F)F)c1

Mol. weight [g/mol]: 263.23

Physical Properties

Property code	Value	Unit	Source
gf	-675.06	kJ/mol	Joback Method
hf	-935.00	kJ/mol	Joback Method
hfus	28.18	kJ/mol	Joback Method
hvap	54.14	kJ/mol	Joback Method
log10ws	-4.27		Crippen Method
logp	3.230		Crippen Method
mcvol	174.810	ml/mol	McGowan Method
pc	2171.40	kPa	Joback Method
rinpol	1479.00		NIST Webbook
rinpol	1479.00		NIST Webbook
tb	608.05	K	Joback Method
tc	797.38	K	Joback Method
tf	368.83	K	Joback Method
vc	0.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	455.31	J/mol×K	608.05	Joback Method
cpg	468.42	J/mol×K	639.60	Joback Method
cpg	480.73	J/mol×K	671.16	Joback Method
cpg	492.26	J/mol×K	702.71	Joback Method
cpg	503.05	J/mol×K	734.27	Joback Method
cpg	513.14	J/mol×K	765.82	Joback Method
cpg	522.58	J/mol×K	797.38	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=U407850&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