Benzamide, 6-trifluoromethyl-2-fluoro-N-(3-methylbutyl)-

Inchi: InChI=1S/C13H15F4NO/c1-8(2)6-7-18-12(19)11-9(13(15,16)17)4-3-5-10(11)14/h3-5,8H,

InchiKey: VDYAUPIKGJUBHN-UHFFFAOYSA-N

Formula: C13H15F4NO

SMILES: CC(C)CCNC(=O)c1c(F)cccc1C(F)(F)F

Mol. weight [g/mol]: 277.26

Physical Properties

Property code	Value	Unit	Source
gf	-666.64	kJ/mol	Joback Method
hf	-955.64	kJ/mol	Joback Method
hfus	30.77	kJ/mol	Joback Method
hvap	56.36	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	3.620		Crippen Method
mcvol	188.900	ml/mol	McGowan Method
pc	1989.43	kPa	Joback Method
rinpol	1637.00		NIST Webbook
rinpol	1637.00		NIST Webbook
tb	630.93	K	Joback Method
tc	818.32	K	Joback Method
tf	380.10	K	Joback Method
vc	0.751	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	505.26	J/mol×K	630.93	Joback Method
cpg	518.90	J/mol×K	662.16	Joback Method
cpg	531.70	J/mol×K	693.39	Joback Method
cpg	543.72	J/mol×K	724.62	Joback Method
cpg	554.98	J/mol×K	755.85	Joback Method
cpg	565.54	J/mol×K	787.08	Joback Method
cpg	575.42	J/mol×K	818.32	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=U407774&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