

Benzamide, 3-fluoro-4-trifluoromethyl-N-(3-methylbutyl)-

Inchi:	InChI=1S/C13H15F4NO/c1-8(2)5-6-18-12(19)9-3-4-10(11(14)7-9)13(15,16)17/h3-4,7-8H
InchiKey:	YUEKSMOMDUKMFY-UHFFFAOYSA-N
Formula:	C13H15F4NO
SMILES:	CC(C)CCNC(=O)c1ccc(C(F)(F)F)c(F)c1
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	1670.00		NIST Webbook
rinpol	1670.00		NIST Webbook
tb	630.93	K	Joback Method
tc	818.32	K	Joback Method
tf	380.10	K	Joback Method
vc	0.751	m ³ /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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407887&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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