

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

Inchi:	InChI=1S/C12H13F4NO/c1-2-3-7-17-11(18)8-5-4-6-9(10(8)13)12(14,15)16/h4-6H,2-3,7H
InchiKey:	PBEBNJGBTUDJIQ-UHFFFAOYSA-N
Formula:	C12H13F4NO
SMILES:	CCCCNC(=O)c1cccc(C(F)(F)F)c1F
Mol. weight [g/mol]:	263.23

Physical Properties

Property code	Value	Unit	Source
gf	-672.62	kJ/mol	Joback Method
hf	-929.72	kJ/mol	Joback Method
hfus	31.70	kJ/mol	Joback Method
hvap	54.52	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	3.374		Crippen Method
mvol	174.810	ml/mol	McGowan Method
pc	2155.30	kPa	Joback Method
rinpol	1533.00		NIST Webbook
rinpol	1533.00		NIST Webbook
tb	608.49	K	Joback Method
tc	794.47	K	Joback Method
tf	383.83	K	Joback Method
vc	0.702	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	454.87	J/molxK	608.49	Joback Method
cpg	467.71	J/molxK	639.49	Joback Method
cpg	479.77	J/molxK	670.48	Joback Method
cpg	491.09	J/molxK	701.48	Joback Method
cpg	501.71	J/molxK	732.47	Joback Method
cpg	511.67	J/molxK	763.47	Joback Method
cpg	520.99	J/molxK	794.47	Joback Method

Sources

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=U407701&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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