

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

Inchi:	InChI=1S/C19H30FNO/c1-4-7-10-16(6-3)15-21(13-8-5-2)19(22)17-11-9-12-18(20)14-17/
InchiKey:	MHTUHORDUBIZLL-UHFFFAOYSA-N
Formula:	C19H30FNO
SMILES:	CCCCC(CC)CN(CCCC)C(=O)c1cccc(F)c1
Mol. weight [g/mol]:	307.45

Physical Properties

Property code	Value	Unit	Source
gf	-3.51	kJ/mol	Joback Method
hf	-456.87	kJ/mol	Joback Method
hfus	42.79	kJ/mol	Joback Method
hvap	68.41	kJ/mol	Joback Method
log10ws	-5.89		Crippen Method
logp	5.284		Crippen Method
mcvol	268.130	ml/mol	McGowan Method
pc	1369.71	kPa	Joback Method
rinpola	2336.00		NIST Webbook
rinpola	2336.00		NIST Webbook
tb	730.92	K	Joback Method
tc	918.56	K	Joback Method
tf	410.82	K	Joback Method
vc	1.028	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	787.34	J/molxK	730.92	Joback Method
cpg	805.38	J/molxK	762.19	Joback Method
cpg	822.40	J/molxK	793.47	Joback Method
cpg	838.45	J/molxK	824.74	Joback Method
cpg	853.58	J/molxK	856.01	Joback Method
cpg	867.84	J/molxK	887.29	Joback Method
cpg	881.26	J/molxK	918.56	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=U415867&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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