

Benzamide, 3-fluoro-N-butyl-N-hexyl-

Inchi:	InChI=1S/C17H26FNO/c1-3-5-7-8-13-19(12-6-4-2)17(20)15-10-9-11-16(18)14-15/h9-11,
InchiKey:	NDYRAXQVILGXNL-UHFFFAOYSA-N
Formula:	C17H26FNO
SMILES:	CCCCCN(CCCC)C(=O)c1cccc(F)c1
Mol. weight [g/mol]:	279.39

Physical Properties

Property code	Value	Unit	Source
gf	-17.91	kJ/mol	Joback Method
hf	-410.31	kJ/mol	Joback Method
hfus	41.14	kJ/mol	Joback Method
hvap	64.35	kJ/mol	Joback Method
log10ws	-5.30		Crippen Method
logp	4.648		Crippen Method
mvol	239.950	ml/mol	McGowan Method
pc	1577.21	kPa	Joback Method
rinpol	2370.00		NIST Webbook
rinpol	2370.00		NIST Webbook
tb	685.60	K	Joback Method
tc	872.34	K	Joback Method
tf	403.28	K	Joback Method
vc	0.921	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	673.63	J/mol×K	685.60	Joback Method
cpg	690.84	J/mol×K	716.72	Joback Method
cpg	707.11	J/mol×K	747.85	Joback Method
cpg	722.46	J/mol×K	778.97	Joback Method
cpg	736.95	J/mol×K	810.09	Joback Method
cpg	750.61	J/mol×K	841.21	Joback Method
cpg	763.48	J/mol×K	872.34	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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=U415866&Units=SI

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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