

Benzamide, 2-fluoro-N-ethyl-N-pentyl-

Inchi:	InChI=1S/C14H20FNO/c1-3-5-8-11-16(4-2)14(17)12-9-6-7-10-13(12)15/h6-7,9-10H,3-5,8
InchiKey:	MOZBJNIRQTZYLK-UHFFFAOYSA-N
Formula:	C14H20FNO
SMILES:	CCCCCN(CC)C(=O)c1ccccc1F
Mol. weight [g/mol]:	237.31

Physical Properties

Property code	Value	Unit	Source
gf	-43.17	kJ/mol	Joback Method
hf	-348.39	kJ/mol	Joback Method
hfus	33.37	kJ/mol	Joback Method
hvap	57.67	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	3.478		Crippen Method
mvol	197.680	ml/mol	McGowan Method
pc	2010.90	kPa	Joback Method
rinpol	1944.00		NIST Webbook
rinpol	1944.00		NIST Webbook
tb	616.96	K	Joback Method
tc	808.81	K	Joback Method
tf	369.47	K	Joback Method
vc	0.753	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	512.73	J/mol×K	616.96	Joback Method
cpg	528.82	J/mol×K	648.94	Joback Method
cpg	544.01	J/mol×K	680.91	Joback Method
cpg	558.33	J/mol×K	712.89	Joback Method
cpg	571.82	J/mol×K	744.86	Joback Method
cpg	584.52	J/mol×K	776.84	Joback Method
cpg	596.46	J/mol×K	808.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415375&Units=SI
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

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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