Benzamide, 2-fluoro-N-hexyl-

Inchi: InChI=1S/C13H18FNO/c1-2-3-4-7-10-15-13(16)11-8-5-6-9-12(11)14/h5-6,8-9H,2-4,7,10H
InchiKey: ZJHXEIONJGUANU-UHFFFAOYSA-N
Formula: C13H18FNO
SMILES: CCCCCCNC(=O)c1ccccc1F
Mol. weight [g/mol]: 223.29

Physical Properties

Property code	Value	Unit	Source
gf	-72.98	kJ/mol	Joback Method
hf	-341.81	kJ/mol	Joback Method
hfus	32.86	kJ/mol	Joback Method
hvap	59.84	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	3.136		Crippen Method
mcvol	183.590	ml/mol	McGowan Method
pc	2227.09	kPa	Joback Method
rinpol	1793.00		NIST Webbook
rinpol	1793.00		NIST Webbook
tb	631.81	K	Joback Method
tc	829.04	K	Joback Method
tf	378.39	K	Joback Method
vc	0.715	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	478.02	J/mol×K	631.81	Joback Method
cpg	492.86	J/mol×K	664.68	Joback Method
cpg	506.85	J/mol×K	697.55	Joback Method
cpg	520.02	J/mol×K	730.43	Joback Method
cpg	532.41	J/mol×K	763.30	Joback Method
cpg	544.06	J/mol×K	796.17	Joback Method
cpg	554.98	J/mol×K	829.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407135&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume