Benzamide, 2-fluoro-N-ethyl-N-hexyl-

Inchi: InChI=1S/C15H22FNO/c1-3-5-6-9-12-17(4-2)15(18)13-10-7-8-11-14(13)16/h7-8,10-11H,
InchiKey: RIVAFBKULSKXQV-UHFFFAOYSA-N
Formula: C15H22FNO
SMILES: CCCCCCN(CC)C(=O)c1ccccc1F
Mol. weight [g/mol]: 251.34

Physical Properties

Property code	Value	Unit	Source
gf	-34.75	kJ/mol	Joback Method
hf	-369.03	kJ/mol	Joback Method
hfus	35.96	kJ/mol	Joback Method
hvap	59.89	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	3.868		Crippen Method
mcvol	211.770	ml/mol	McGowan Method
pc	1848.33	kPa	Joback Method
rinpol	2027.00		NIST Webbook
rinpol	2027.00		NIST Webbook
tb	639.84	K	Joback Method
tc	829.64	K	Joback Method
tf	380.74	K	Joback Method
vc	0.809	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	565.06	J/mol×K	639.84	Joback Method
cpg	581.58	J/mol×K	671.47	Joback Method
cpg	597.17	J/mol×K	703.11	Joback Method
cpg	611.88	J/mol×K	734.74	Joback Method
cpg	625.75	J/mol×K	766.37	Joback Method
cpg	638.81	J/mol×K	798.01	Joback Method
cpg	651.11	J/mol×K	829.64	Joback Method

Sources

Crippen Method:	https://www.chemeo.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=U415377&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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