Benzamide, 2-fluoro-N-ethyl-N-heptyl-

Inchi: InChI=1S/C16H24FNO/c1-3-5-6-7-10-13-18(4-2)16(19)14-11-8-9-12-15(14)17/h8-9,11-12
InchiKey: XDQFLRZQRGJQEL-UHFFFAOYSA-N
Formula: C16H24FNO
SMILES: CCCCCCCN(CC)C(=O)c1ccccc1F
Mol. weight [g/mol]: 265.37

Physical Properties

Property code	Value	Unit	Source
gf	-26.33	kJ/mol	Joback Method
hf	-389.67	kJ/mol	Joback Method
hfus	38.55	kJ/mol	Joback Method
hvap	62.12	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	4.258		Crippen Method
mcvol	225.860	ml/mol	McGowan Method
pc	1704.71	kPa	Joback Method
rinpol	2152.00		NIST Webbook
rinpol	2152.00		NIST Webbook
tb	662.72	K	Joback Method
tc	850.80	K	Joback Method
tf	392.01	K	Joback Method
vc	0.866	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	618.72	J/mol×K	662.72	Joback Method
cpg	635.61	J/mol×K	694.07	Joback Method
cpg	651.56	J/mol×K	725.41	Joback Method
cpg	666.61	J/mol×K	756.76	Joback Method
cpg	680.81	J/mol×K	788.11	Joback Method
cpg	694.19	J/mol×K	819.45	Joback Method
cpg	706.79	J/mol×K	850.80	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=U415379&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