Benzamide, 3-fluoro-N-nonyl-

Inchi: InChI=1S/C16H24FNO/c1-2-3-4-5-6-7-8-12-18-16(19)14-10-9-11-15(17)13-14/h9-11,13H
InchiKey: KTULKXGWYAEJQP-UHFFFAOYSA-N
Formula: C16H24FNO
SMILES: CCCCCCCCCNC(=O)c1cccc(F)c1
Mol. weight [g/mol]: 265.37

Physical Properties

Property code	Value	Unit	Source
gf	-47.72	kJ/mol	Joback Method
hf	-403.73	kJ/mol	Joback Method
hfus	40.63	kJ/mol	Joback Method
hvap	66.51	kJ/mol	Joback Method
log10ws	-5.50		Crippen Method
logp	4.306		Crippen Method
mcvol	225.860	ml/mol	McGowan Method
pc	1726.03	kPa	Joback Method
rinpol	2158.00		NIST Webbook
rinpol	2158.00		NIST Webbook
tb	700.45	K	Joback Method
tc	891.83	K	Joback Method
tf	412.20	K	Joback Method
vc	0.882	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	637.14	J/mol×K	700.45	Joback Method
cpg	653.25	J/mol×K	732.35	Joback Method
cpg	668.46	J/mol×K	764.24	Joback Method
cpg	682.79	J/mol×K	796.14	Joback Method
cpg	696.29	J/mol×K	828.04	Joback Method
cpg	708.99	J/mol×K	859.93	Joback Method
cpg	720.92	J/mol×K	891.83	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407286&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