Benzamide, 3,4-difluoro-N-hexyl-

Inchi: InChI=1S/C13H17F2NO/c1-2-3-4-5-8-16-13(17)10-6-7-11(14)12(15)9-10/h6-7,9H,2-5,8H
InchiKey: QCLOBVWKXCHRMW-UHFFFAOYSA-N
Formula: C13H17F2NO
SMILES: CCCCCCNC(=O)c1ccc(F)c(F)c1
Mol. weight [g/mol]: 241.28

Physical Properties

Property code	Value	Unit	Source
gf	-277.42	kJ/mol	Joback Method
hf	-549.39	kJ/mol	Joback Method
hfus	35.55	kJ/mol	Joback Method
hvap	59.68	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	3.275		Crippen Method
mcvol	185.360	ml/mol	McGowan Method
pc	2106.13	kPa	Joback Method
rinpol	1830.00		NIST Webbook
rinpol	1830.00		NIST Webbook
tb	636.06	K	Joback Method
tc	826.22	K	Joback Method
tf	391.50	K	Joback Method
vc	0.733	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.55	J/mol×K	636.06	Joback Method
cpg	499.57	J/mol×K	667.75	Joback Method
cpg	512.82	J/mol×K	699.45	Joback Method
cpg	525.34	J/mol×K	731.14	Joback Method
cpg	537.15	J/mol×K	762.83	Joback Method
cpg	548.27	J/mol×K	794.52	Joback Method
cpg	558.73	J/mol×K	826.22	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407794&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