Benzamide, 3,4-difluoro-N-undecyl-

Inchi: InChI=1S/C18H27F2NO/c1-2-3-4-5-6-7-8-9-10-13-21-18(22)15-11-12-16(19)17(20)14-15
InchiKey: UQYLZFPBFITFTF-UHFFFAOYSA-N
Formula: C18H27F2NO
SMILES: CCCCCCCCCCCNC(=O)c1ccc(F)c(F)c1
Mol. weight [g/mol]: 311.41

Physical Properties

Property code	Value	Unit	Source
gf	-235.32	kJ/mol	Joback Method
hf	-652.59	kJ/mol	Joback Method
hfus	48.50	kJ/mol	Joback Method
hvap	70.81	kJ/mol	Joback Method
log10ws	-6.67		Crippen Method
logp	5.225		Crippen Method
mcvol	255.810	ml/mol	McGowan Method
pc	1414.37	kPa	Joback Method
rinpol	2353.00		NIST Webbook
rinpol	2353.00		NIST Webbook
tb	750.46	K	Joback Method
tc	935.88	K	Joback Method
tf	447.85	K	Joback Method
vc	1.012	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	756.51	J/mol×K	750.46	Joback Method
cpg	772.66	J/mol×K	781.36	Joback Method
cpg	787.91	J/mol×K	812.27	Joback Method
cpg	802.31	J/mol×K	843.17	Joback Method
cpg	815.89	J/mol×K	874.08	Joback Method
cpg	828.68	J/mol×K	904.98	Joback Method
cpg	840.71	J/mol×K	935.88	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=U407800&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