Benzamide, 2,6-difluoro-3-methyl-N-undecyl-

Inchi: InChI=1S/C19H29F2NO/c1-3-4-5-6-7-8-9-10-11-14-22-19(23)17-16(20)13-12-15(2)18(17
InchiKey: IPLIDSQZCXYXLN-UHFFFAOYSA-N
Formula: C19H29F2NO
SMILES: CCCCCCCCCCCNC(=O)c1c(F)ccc(C)c1F
Mol. weight [g/mol]: 325.44

Physical Properties

Property code	Value	Unit	Source
gf	-236.53	kJ/mol	Joback Method
hf	-684.70	kJ/mol	Joback Method
hfus	50.70	kJ/mol	Joback Method
hvap	73.70	kJ/mol	Joback Method
log10ws	-7.14		Crippen Method
logp	5.534		Crippen Method
mcvol	269.900	ml/mol	McGowan Method
pc	1303.29	kPa	Joback Method
rinpol	2475.00		NIST Webbook
rinpol	2475.00		NIST Webbook
tb	778.32	K	Joback Method
tc	965.18	K	Joback Method
tf	471.64	K	Joback Method
vc	1.069	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	813.67	J/mol×K	778.32	Joback Method
cpg	830.09	J/mol×K	809.46	Joback Method
cpg	845.61	J/mol×K	840.61	Joback Method
cpg	860.25	J/mol×K	871.75	Joback Method
cpg	874.04	J/mol×K	902.89	Joback Method
cpg	887.01	J/mol×K	934.03	Joback Method
cpg	899.21	J/mol×K	965.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407747&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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