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

Inchi: InChI=1S/C12H15F2NO/c1-3-4-7-15-12(16)10-9(13)6-5-8(2)11(10)14/h5-6H,3-4,7H2,1-2
InchiKey: ZCCNMOWICAHCFV-UHFFFAOYSA-N
Formula: C12H15F2NO
SMILES: CCCCNC(=O)c1c(F)ccc(C)c1F
Mol. weight [g/mol]: 227.25

Physical Properties

Property code	Value	Unit	Source
gf	-295.47	kJ/mol	Joback Method
hf	-540.22	kJ/mol	Joback Method
hfus	32.57	kJ/mol	Joback Method
hvap	58.12	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	2.803		Crippen Method
mcvol	171.270	ml/mol	McGowan Method
pc	2271.90	kPa	Joback Method
rinpol	1740.00		NIST Webbook
rinpol	1740.00		NIST Webbook
tb	618.16	K	Joback Method
tc	811.33	K	Joback Method
tf	392.75	K	Joback Method
vc	0.676	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	434.72	J/mol×K	618.16	Joback Method
cpg	447.95	J/mol×K	650.35	Joback Method
cpg	460.49	J/mol×K	682.55	Joback Method
cpg	472.35	J/mol×K	714.74	Joback Method
cpg	483.55	J/mol×K	746.94	Joback Method
cpg	494.11	J/mol×K	779.13	Joback Method
cpg	504.05	J/mol×K	811.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407737&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