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

Inchi: InChI=1S/C9H9F2NO/c1-5-3-4-6(10)7(8(5)11)9(13)12-2/h3-4H,1-2H3,(H,12,13)
InchiKey: YFKOGSSJHGZKLC-UHFFFAOYSA-N
Formula: C9H9F2NO
SMILES: CNC(=O)c1c(F)ccc(C)c1F
Mol. weight [g/mol]: 185.17

Physical Properties

Property code	Value	Unit	Source
gf	-320.73	kJ/mol	Joback Method
hf	-478.30	kJ/mol	Joback Method
hfus	24.80	kJ/mol	Joback Method
hvap	51.44	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	1.633		Crippen Method
mcvol	129.000	ml/mol	McGowan Method
pc	3052.41	kPa	Joback Method
rinpol	1502.00		NIST Webbook
rinpol	1502.00		NIST Webbook
tb	549.52	K	Joback Method
tc	750.58	K	Joback Method
tf	358.94	K	Joback Method
vc	0.508	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	293.56	J/mol×K	549.52	Joback Method
cpg	304.42	J/mol×K	583.03	Joback Method
cpg	314.72	J/mol×K	616.54	Joback Method
cpg	324.45	J/mol×K	650.05	Joback Method
cpg	333.64	J/mol×K	683.56	Joback Method
cpg	342.30	J/mol×K	717.07	Joback Method
cpg	350.44	J/mol×K	750.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407733&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