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

Inchi: InChI=1S/C13H17F2NO/c1-8(2)6-7-16-13(17)11-10(14)5-4-9(3)12(11)15/h4-5,8H,6-7H2,

InchiKey: BXZVTWXFNMPXOI-UHFFFAOYSA-N

Formula: C13H17F2NO

SMILES: Cc1ccc(F)c(C(=O)NCCC(C)C)c1F

Mol. weight [g/mol]: 241.28

Physical Properties

Property code	Value	Unit	Source
gf	-289.49	kJ/mol	Joback Method
hf	-566.14	kJ/mol	Joback Method
hfus	31.64	kJ/mol	Joback Method
hvap	59.95	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	3.049		Crippen Method
mcvol	185.360	ml/mol	McGowan Method
pc	2092.66	kPa	Joback Method
rinpol	1799.00		NIST Webbook
rinpol	1799.00		NIST Webbook
tb	640.60	K	Joback Method
tc	834.97	K	Joback Method
tf	389.02	K	Joback Method
vc	0.727	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.44	J/mol×K	640.60	Joback Method
cpg	499.56	J/mol×K	673.00	Joback Method
cpg	512.91	J/mol×K	705.39	Joback Method
cpg	525.53	J/mol×K	737.79	Joback Method
cpg	537.42	J/mol×K	770.18	Joback Method
cpg	548.61	J/mol×K	802.58	Joback Method
cpg	559.12	J/mol×K	834.97	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407738&Units=SI

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