Benzamide, 2,5-difluoro-N-butyl-

Inchi: InChI=1S/C11H13F2NO/c1-2-3-6-14-11(15)9-7-8(12)4-5-10(9)13/h4-5,7H,2-3,6H2,1H3,(
InchiKey: ZJSFQQYNFGQSRX-UHFFFAOYSA-N
Formula: C11H13F2NO
SMILES: CCCCNC(=O)c1cc(F)ccc1F
Mol. weight [g/mol]: 213.22

Physical Properties

Property code	Value	Unit	Source
gf	-294.26	kJ/mol	Joback Method
hf	-508.11	kJ/mol	Joback Method
hfus	30.37	kJ/mol	Joback Method
hvap	55.23	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	2.495		Crippen Method
mcvol	157.180	ml/mol	McGowan Method
pc	2532.82	kPa	Joback Method
rinpol	1546.00		NIST Webbook
tb	590.30	K	Joback Method
tc	784.94	K	Joback Method
tf	368.96	K	Joback Method
vc	0.621	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	386.60	J/mol×K	590.30	Joback Method
cpg	399.37	J/mol×K	622.74	Joback Method
cpg	411.45	J/mol×K	655.18	Joback Method
cpg	422.84	J/mol×K	687.62	Joback Method
cpg	433.58	J/mol×K	720.06	Joback Method
cpg	443.69	J/mol×K	752.50	Joback Method
cpg	453.18	J/mol×K	784.94	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=U407584&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