Benzamide, N,N-dibutyl-2,6-difluoro-

Inchi: InChI=1S/C15H21F2NO/c1-3-5-10-18(11-6-4-2)15(19)14-12(16)8-7-9-13(14)17/h7-9H,3-
InchiKey: BTXNGJCNHCDPDU-UHFFFAOYSA-N
Formula: C15H21F2NO
SMILES: CCCCN(CCCC)C(=O)c1c(F)cccc1F
Mol. weight [g/mol]: 269.33

Physical Properties

Property code	Value	Unit	Source
gf	-239.19	kJ/mol	Joback Method
hf	-576.61	kJ/mol	Joback Method
hfus	38.65	kJ/mol	Joback Method
hvap	59.74	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	4.007		Crippen Method
mcvol	213.540	ml/mol	McGowan Method
pc	1756.54	kPa	Joback Method
rinpol	1713.00		NIST Webbook
tb	644.09	K	Joback Method
tc	827.59	K	Joback Method
tf	393.85	K	Joback Method
vc	0.828	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.85	J/mol×K	644.09	Joback Method
cpg	588.53	J/mol×K	674.67	Joback Method
cpg	603.36	J/mol×K	705.26	Joback Method
cpg	617.40	J/mol×K	735.84	Joback Method
cpg	630.66	J/mol×K	766.42	Joback Method
cpg	643.18	J/mol×K	797.01	Joback Method
cpg	654.99	J/mol×K	827.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308664&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

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