Benzamide, 2,5-difluoro-N-(2,5-difluorobenzoyl)-N-butyl-

Inchi: InChI=1S/C18H15F4NO2/c1-2-3-8-23(17(24)13-9-11(19)4-6-15(13)21)18(25)14-10-12(20

InchiKey: YVBFQUQUZPXOMS-UHFFFAOYSA-N

Formula: C18H15F4NO2

SMILES: CCCCN(C(=O)c1cc(F)ccc1F)C(=O)c1cc(F)ccc1F

Mol. weight [g/mol]: 353.31

Physical Properties

Property code	Value	Unit	Source
gf	-639.32	kJ/mol	Joback Method
hf	-929.74	kJ/mol	Joback Method
hfus	47.44	kJ/mol	Joback Method
hvap	75.13	kJ/mol	Joback Method
log10ws	-6.16		Crippen Method
logp	4.326		Crippen Method
mcvol	237.160	ml/mol	McGowan Method
pc	1736.11	kPa	Joback Method
rinpol	2029.00		NIST Webbook
rinpol	2029.00		NIST Webbook
tb	801.78	K	Joback Method
tc	1005.53	K	Joback Method
tf	530.23	K	Joback Method
vc	0.929	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	682.01	J/mol×K	801.78	Joback Method
cpg	694.56	J/mol×K	835.74	Joback Method
cpg	706.19	J/mol×K	869.70	Joback Method
cpg	716.94	J/mol×K	903.65	Joback Method
cpg	726.87	J/mol×K	937.61	Joback Method
cpg	736.01	J/mol×K	971.57	Joback Method
cpg	744.42	J/mol×K	1005.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407602&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