Benzamide, 2,4-difluoro-N-(2,4-difluorobenzoyl)-N-isobutyl-

Inchi: InChI=1S/C18H15F4NO2/c1-10(2)9-23(17(24)13-5-3-11(19)7-15(13)21)18(25)14-6-4-12(

InchiKey: PYLDFOKVVNRJRK-UHFFFAOYSA-N

Formula: C18H15F4NO2

SMILES: CC(C)CN(C(=O)c1ccc(F)cc1F)C(=O)c1ccc(F)cc1F

Mol. weight [g/mol]: 353.31

Physical Properties

Property code	Value	Unit	Source
gf	-641.76	kJ/mol	Joback Method
hf	-935.02	kJ/mol	Joback Method
hfus	43.92	kJ/mol	Joback Method
hvap	74.74	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	4.182		Crippen Method
mcvol	237.160	ml/mol	McGowan Method
pc	1747.74	kPa	Joback Method
rinpol	1965.00		NIST Webbook
rinpol	1965.00		NIST Webbook
tb	801.34	K	Joback Method
tc	1007.61	K	Joback Method
tf	515.23	K	Joback Method
vc	0.923	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	682.60	J/mol×K	801.34	Joback Method
cpg	695.29	J/mol×K	835.72	Joback Method
cpg	707.04	J/mol×K	870.10	Joback Method
cpg	717.88	J/mol×K	904.48	Joback Method
cpg	727.86	J/mol×K	938.86	Joback Method
cpg	737.03	J/mol×K	973.23	Joback Method
cpg	745.44	J/mol×K	1007.61	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=U407620&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