Benzamide, 2,6-difluoro-3-methyl-N-(2,6-difluoro-3-methylbenz

Inchi: InChI=1S/C18H15F4NO2/c1-4-23(17(24)13-11(19)7-5-9(2)15(13)21)18(25)14-12(20)8-6-

InchiKey: VHOFRQGMWWPGQG-UHFFFAOYSA-N

Formula: C18H15F4NO2

SMILES: CCN(C(=O)c1c(F)ccc(C)c1F)C(=O)c1c(F)ccc(C)c1F

Mol. weight [g/mol]: 353.31

Physical Properties

Property code	Value	Unit	Source
gf	-658.58	kJ/mol	Joback Method
hf	-952.68	kJ/mol	Joback Method
hfus	46.66	kJ/mol	Joback Method
hvap	76.45	kJ/mol	Joback Method
log10ws	-6.28		Crippen Method
logp	4.162		Crippen Method
mcvol	237.160	ml/mol	McGowan Method
pc	1693.51	kPa	Joback Method
rinpol	2130.00		NIST Webbook
rinpol	2130.00		NIST Webbook
tb	811.74	K	Joback Method
tc	1017.10	K	Joback Method
tf	555.27	K	Joback Method
vc	0.929	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	679.54	J/mol×K	811.74	Joback Method
cpg	691.93	J/mol×K	845.97	Joback Method
cpg	703.41	J/mol×K	880.19	Joback Method
cpg	714.03	J/mol×K	914.42	Joback Method
cpg	723.82	J/mol×K	948.65	Joback Method
cpg	732.81	J/mol×K	982.87	Joback Method
cpg	741.04	J/mol×K	1017.10	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407753&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