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

Inchi: InChI=1S/C22H23F4NO2/c1-4-5-6-7-12-27(21(28)17-15(23)10-8-13(2)19(17)25)22(29)18

InchiKey: IKRSWCRFDKFHDW-UHFFFAOYSA-N

Formula: C22H23F4NO2

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

Mol. weight [g/mol]: 409.42

Physical Properties

Property code	Value	Unit	Source
gf	-624.90	kJ/mol	Joback Method
hf	-1035.24	kJ/mol	Joback Method
hfus	57.02	kJ/mol	Joback Method
hvap	85.36	kJ/mol	Joback Method
log10ws	-7.95		Crippen Method
logp	5.723		Crippen Method
mcvol	293.520	ml/mol	McGowan Method
pc	1262.85	kPa	Joback Method
rinpol	2502.00		NIST Webbook
rinpol	2502.00		NIST Webbook
tb	903.26	K	Joback Method
tc	1110.94	K	Joback Method
tf	600.35	K	Joback Method
vc	1.153	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	907.81	J/mol×K	903.26	Joback Method
cpg	921.45	J/mol×K	937.87	Joback Method
cpg	934.06	J/mol×K	972.49	Joback Method
cpg	945.69	J/mol×K	1007.10	Joback Method
cpg	956.40	J/mol×K	1041.71	Joback Method
cpg	966.22	J/mol×K	1076.32	Joback Method
cpg	975.21	J/mol×K	1110.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407760&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