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

Inchi: InChI=1S/C27H33F4NO2/c1-4-5-6-7-8-9-10-11-12-17-32(26(33)22-20(28)15-13-18(2)24(

InchiKey: ANMKITBTGBMSNA-UHFFFAOYSA-N

Formula: C27H33F4NO2

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

Mol. weight [g/mol]: 479.55

Physical Properties

Property code	Value	Unit	Source
gf	-582.80	kJ/mol	Joback Method
hf	-1138.44	kJ/mol	Joback Method
hfus	69.97	kJ/mol	Joback Method
hvap	96.49	kJ/mol	Joback Method
log10ws	-10.05		Crippen Method
logp	7.673		Crippen Method
mcvol	363.970	ml/mol	McGowan Method
pc	921.62	kPa	Joback Method
rinpol	3019.00		NIST Webbook
tb	1017.66	K	Joback Method
tc	1247.60	K	Joback Method
tf	656.70	K	Joback Method
vc	1.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1208.92	J/mol×K	1017.66	Joback Method
cpg	1224.35	J/mol×K	1055.98	Joback Method
cpg	1238.49	J/mol×K	1094.31	Joback Method
cpg	1251.41	J/mol×K	1132.63	Joback Method
cpg	1263.20	J/mol×K	1170.95	Joback Method
cpg	1273.95	J/mol×K	1209.27	Joback Method
cpg	1283.73	J/mol×K	1247.60	Joback Method

Sources

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=U407764&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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