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

Inchi: InChI=1S/C21H21F4NO2/c1-11(2)9-10-26(20(27)16-14(22)7-5-12(3)18(16)24)21(28)17-1

InchiKey: JDILZXLEFSEZDS-UHFFFAOYSA-N

Formula: C21H21F4NO2

SMILES: Cc1ccc(F)c(C(=O)N(CCC(C)C)C(=O)c2c(F)ccc(C)c2F)c1F

Mol. weight [g/mol]: 395.39

Physical Properties

Property code	Value	Unit	Source
gf	-635.76	kJ/mol	Joback Method
hf	-1019.88	kJ/mol	Joback Method
hfus	50.91	kJ/mol	Joback Method
hvap	82.74	kJ/mol	Joback Method
log10ws	-7.29		Crippen Method
logp	5.189		Crippen Method
mcvol	279.430	ml/mol	McGowan Method
pc	1361.64	kPa	Joback Method
rinpol	2350.00		NIST Webbook
rinpol	2350.00		NIST Webbook
tb	879.94	K	Joback Method
tc	1087.46	K	Joback Method
tf	574.08	K	Joback Method
vc	1.091	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	850.05	J/mol×K	879.94	Joback Method
cpg	863.46	J/mol×K	914.53	Joback Method
cpg	875.85	J/mol×K	949.11	Joback Method
cpg	887.27	J/mol×K	983.70	Joback Method
cpg	897.77	J/mol×K	1018.29	Joback Method
cpg	907.38	J/mol×K	1052.88	Joback Method
cpg	916.16	J/mol×K	1087.46	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=U407757&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