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

Inchi: InChI=1S/C23H25F4NO2/c1-5-6-7-8-15(4)28(22(29)18-16(24)11-9-13(2)20(18)26)23(30)

InchiKey: XTRUZBVBYDPPGG-UHFFFAOYSA-N

Formula: C23H25F4NO2

SMILES: CCCCCC(C)N(C(=O)c1c(F)ccc(C)c1F)C(=O)c1c(F)ccc(C)c1F

Mol. weight [g/mol]: 423.44

Physical Properties

Property code	Value	Unit	Source
gf	-618.92	kJ/mol	Joback Method
hf	-1061.16	kJ/mol	Joback Method
hfus	56.09	kJ/mol	Joback Method
hvap	87.20	kJ/mol	Joback Method
log10ws	-8.48		Crippen Method
logp	6.111		Crippen Method
mcvol	307.610	ml/mol	McGowan Method
pc	1187.42	kPa	Joback Method
rinpol	2525.00		NIST Webbook
rinpol	2525.00		NIST Webbook
tb	925.70	K	Joback Method
tc	1136.74	K	Joback Method
tf	596.62	K	Joback Method
vc	1.204	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	967.29	J/mol×K	925.70	Joback Method
cpg	981.25	J/mol×K	960.87	Joback Method
cpg	994.13	J/mol×K	996.05	Joback Method
cpg	1005.98	J/mol×K	1031.22	Joback Method
cpg	1016.84	J/mol×K	1066.39	Joback Method
cpg	1026.78	J/mol×K	1101.57	Joback Method
cpg	1035.84	J/mol×K	1136.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407759&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