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

Inchi: InChI=1S/C21H21F4NO2/c1-4-5-6-11-26(20(27)16-14(22)9-7-12(2)18(16)24)21(28)17-15

InchiKey: MCDUGIICDYZWAP-UHFFFAOYSA-N

Formula: C21H21F4NO2

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

Mol. weight [g/mol]: 395.39

Physical Properties

Property code	Value	Unit	Source
gf	-633.32	kJ/mol	Joback Method
hf	-1014.60	kJ/mol	Joback Method
hfus	54.43	kJ/mol	Joback Method
hvap	83.13	kJ/mol	Joback Method
log10ws	-7.53		Crippen Method
logp	5.333		Crippen Method
mcvol	279.430	ml/mol	McGowan Method
pc	1353.63	kPa	Joback Method
rinpol	2398.00		NIST Webbook
rinpol	2398.00		NIST Webbook
tb	880.38	K	Joback Method
tc	1086.37	K	Joback Method
tf	589.08	K	Joback Method
vc	1.097	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	849.52	J/mol×K	880.38	Joback Method
cpg	862.86	J/mol×K	914.71	Joback Method
cpg	875.20	J/mol×K	949.04	Joback Method
cpg	886.60	J/mol×K	983.37	Joback Method
cpg	897.10	J/mol×K	1017.70	Joback Method
cpg	906.74	J/mol×K	1052.03	Joback Method
cpg	915.56	J/mol×K	1086.37	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=U407758&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