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

Inchi: InChI=1S/C30H39F4NO2/c1-4-5-6-7-8-9-10-11-12-13-14-15-20-35(29(36)25-23(31)18-1

InchiKey: BPTSNEZXAMFNCK-UHFFFAOYSA-N

Formula: C30H39F4NO2

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

Mol. weight [g/mol]: 521.63

Physical Properties

Property code	Value	Unit	Source
gf	-557.54	kJ/mol	Joback Method
hf	-1200.36	kJ/mol	Joback Method
hfus	77.74	kJ/mol	Joback Method
hvap	103.17	kJ/mol	Joback Method
log10ws	-11.30		Crippen Method
logp	8.844		Crippen Method
mcvol	406.240	ml/mol	McGowan Method
pc	779.38	kPa	Joback Method
rinpol	3329.00		NIST Webbook
rinpol	3329.00		NIST Webbook
tb	1086.30	K	Joback Method
tc	1343.26	K	Joback Method
tf	690.51	K	Joback Method
vc	1.601	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1395.69	J/mol×K	1086.30	Joback Method
cpg	1412.68	J/mol×K	1129.13	Joback Method
cpg	1428.09	J/mol×K	1171.95	Joback Method
cpg	1442.06	J/mol×K	1214.78	Joback Method
cpg	1454.73	J/mol×K	1257.60	Joback Method
cpg	1466.23	J/mol×K	1300.43	Joback Method
cpg	1476.70	J/mol×K	1343.26	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=U407766&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