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

Inchi: InChI=1S/C28H35F4NO2/c1-4-5-6-7-8-9-10-11-12-13-18-33(27(34)23-21(29)16-14-19(2)

InchiKey: JMRLSLSAZIOUAF-UHFFFAOYSA-N

Formula: C28H35F4NO2

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

Mol. weight [g/mol]: 493.58

Physical Properties

Property code	Value	Unit	Source
gf	-574.38	kJ/mol	Joback Method
hf	-1159.08	kJ/mol	Joback Method
hfus	72.56	kJ/mol	Joback Method
hvap	98.71	kJ/mol	Joback Method
log10ws	-10.47		Crippen Method
logp	8.063		Crippen Method
mcvol	378.060	ml/mol	McGowan Method
pc	870.16	kPa	Joback Method
rinpol	3121.00		NIST Webbook
rinpol	3121.00		NIST Webbook
tb	1040.54	K	Joback Method
tc	1278.18	K	Joback Method
tf	667.97	K	Joback Method
vc	1.490	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1270.74	J/mol×K	1040.54	Joback Method
cpg	1286.65	J/mol×K	1080.15	Joback Method
cpg	1301.17	J/mol×K	1119.75	Joback Method
cpg	1314.40	J/mol×K	1159.36	Joback Method
cpg	1326.46	J/mol×K	1198.96	Joback Method
cpg	1337.42	J/mol×K	1238.57	Joback Method
cpg	1347.41	J/mol×K	1278.18	Joback Method

Sources

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=U407765&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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