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

Inchi: InChI=1S/C32H43F4NO2/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-22-37(31(38)27-25(33

InchiKey: ZCFURJJTWDVNSN-UHFFFAOYSA-N

Formula: C32H43F4NO2

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

Mol. weight [g/mol]: 549.68

Physical Properties

Property code	Value	Unit	Source
gf	-540.70	kJ/mol	Joback Method
hf	-1241.64	kJ/mol	Joback Method
hfus	82.92	kJ/mol	Joback Method
hvap	107.62	kJ/mol	Joback Method
log10ws	-12.14		Crippen Method
logp	9.624		Crippen Method
mcvol	434.420	ml/mol	McGowan Method
pc	702.10	kPa	Joback Method
rinpol	3540.00		NIST Webbook
rinpol	3540.00		NIST Webbook
tb	1132.06	K	Joback Method
tc	1414.24	K	Joback Method
tf	713.05	K	Joback Method
vc	1.714	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1522.15	J/mol×K	1132.06	Joback Method
cpg	1540.48	J/mol×K	1179.09	Joback Method
cpg	1556.99	J/mol×K	1226.12	Joback Method
cpg	1571.87	J/mol×K	1273.15	Joback Method
cpg	1585.33	J/mol×K	1320.18	Joback Method
cpg	1597.55	J/mol×K	1367.21	Joback Method
cpg	1608.74	J/mol×K	1414.24	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=U407767&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