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

Inchi: InChI=1S/C26H31F4NO2/c1-4-5-6-7-8-9-10-11-16-31(25(32)21-19(27)14-12-17(2)23(21)
InchiKey: GIMKXSCYPUKPER-UHFFFAOYSA-N
Formula: C26H31F4NO2
SMILES: CCCCCCCCCCN(C(=O)c1c(F)ccc(C)c1F)C(=O)c1c(F)ccc(C)c1F
Mol. weight [g/mol]: 465.52

Physical Properties

Property code	Value	Unit	Source
gf	-591.22	kJ/mol	Joback Method
hf	-1117.80	kJ/mol	Joback Method
hfus	67.38	kJ/mol	Joback Method
hvap	94.26	kJ/mol	Joback Method
log10ws	-9.63		Crippen Method
logp	7.283		Crippen Method
mcvol	349.880	ml/mol	McGowan Method
pc	977.78	kPa	Joback Method
rinpol	2916.00		NIST Webbook
rinpol	2916.00		NIST Webbook
tb	994.78	K	Joback Method
tc	1218.20	K	Joback Method
tf	645.43	K	Joback Method
vc	1.377	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1147.57	J/mol×K	994.78	Joback Method
cpg	1162.58	J/mol×K	1032.02	Joback Method
cpg	1176.37	J/mol×K	1069.25	Joback Method
cpg	1189.00	J/mol×K	1106.49	Joback Method
cpg	1200.55	J/mol×K	1143.73	Joback Method
cpg	1211.10	J/mol×K	1180.96	Joback Method
cpg	1220.71	J/mol×K	1218.20	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=U407763&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