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

Inchi: InChI=1S/C17H13F4NO2/c1-8-4-6-10(18)12(14(8)20)16(23)22(3)17(24)13-11(19)7-5-9(2

InchiKey: ZDLFNWPIMUYLQF-UHFFFAOYSA-N

Formula: C17H13F4NO2

SMILES: Cc1ccc(F)c(C(=O)N(C)C(=O)c2c(F)ccc(C)c2F)c1F

Mol. weight [g/mol]: 339.28

Physical Properties

Property code	Value	Unit	Source
gf	-667.00	kJ/mol	Joback Method
hf	-932.04	kJ/mol	Joback Method
hfus	44.07	kJ/mol	Joback Method
hvap	74.23	kJ/mol	Joback Method
log10ws	-5.86		Crippen Method
logp	3.772		Crippen Method
mcvol	223.070	ml/mol	McGowan Method
pc	1835.69	kPa	Joback Method
rinpol	2085.00		NIST Webbook
rinpol	2085.00		NIST Webbook
tb	788.86	K	Joback Method
tc	995.33	K	Joback Method
tf	544.00	K	Joback Method
vc	0.874	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	624.71	J/mol×K	788.86	Joback Method
cpg	636.74	J/mol×K	823.27	Joback Method
cpg	647.90	J/mol×K	857.68	Joback Method
cpg	658.21	J/mol×K	892.09	Joback Method
cpg	667.70	J/mol×K	926.50	Joback Method
cpg	676.43	J/mol×K	960.92	Joback Method
cpg	684.40	J/mol×K	995.33	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=U407752&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