Benzamide, 2,5-difluoro-N-(2,5-difluorobenzoyl)-N-(3-methylbu

Inchi: InChI=1S/C19H17F4NO2/c1-11(2)7-8-24(18(25)14-9-12(20)3-5-16(14)22)19(26)15-10-13

InchiKey: OCYNZMVUJTZLCR-UHFFFAOYSA-N

Formula: C19H17F4NO2

SMILES: CC(C)CCN(C(=O)c1cc(F)ccc1F)C(=O)c1cc(F)ccc1F

Mol. weight [g/mol]: 367.34

Physical Properties

Property code	Value	Unit	Source
gf	-633.34	kJ/mol	Joback Method
hf	-955.66	kJ/mol	Joback Method
hfus	46.51	kJ/mol	Joback Method
hvap	76.97	kJ/mol	Joback Method
log10ws	-6.34		Crippen Method
logp	4.572		Crippen Method
mcvol	251.250	ml/mol	McGowan Method
pc	1615.47	kPa	Joback Method
rinpol	2080.00		NIST Webbook
rinpol	2080.00		NIST Webbook
tb	824.22	K	Joback Method
tc	1029.67	K	Joback Method
tf	526.50	K	Joback Method
vc	0.980	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	738.25	J/mol×K	824.22	Joback Method
cpg	751.25	J/mol×K	858.46	Joback Method
cpg	763.28	J/mol×K	892.70	Joback Method
cpg	774.38	J/mol×K	926.94	Joback Method
cpg	784.62	J/mol×K	961.18	Joback Method
cpg	794.03	J/mol×K	995.42	Joback Method
cpg	802.68	J/mol×K	1029.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407603&Units=SI
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

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