Benzamide, 2,4-difluoro-N-(2,4-difluorobenzoyl)-N-pentyl-

Inchi: InChI=1S/C19H17F4NO2/c1-2-3-4-9-24(18(25)14-7-5-12(20)10-16(14)22)19(26)15-8-6-1

InchiKey: GPEAZNLLEQMTLE-UHFFFAOYSA-N

Formula: C19H17F4NO2

SMILES: CCCCCN(C(=O)c1ccc(F)cc1F)C(=O)c1ccc(F)cc1F

Mol. weight [g/mol]: 367.34

Physical Properties

Property code	Value	Unit	Source
gf	-630.90	kJ/mol	Joback Method
hf	-950.38	kJ/mol	Joback Method
hfus	50.03	kJ/mol	Joback Method
hvap	77.36	kJ/mol	Joback Method
log10ws	-6.58		Crippen Method
logp	4.716		Crippen Method
mcvol	251.250	ml/mol	McGowan Method
pc	1605.13	kPa	Joback Method
rinpol	2108.00		NIST Webbook
rinpol	2108.00		NIST Webbook
tb	824.66	K	Joback Method
tc	1027.89	K	Joback Method
tf	541.50	K	Joback Method
vc	0.986	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	737.68	J/mol×K	824.66	Joback Method
cpg	750.55	J/mol×K	858.53	Joback Method
cpg	762.48	J/mol×K	892.40	Joback Method
cpg	773.51	J/mol×K	926.27	Joback Method
cpg	783.71	J/mol×K	960.15	Joback Method
cpg	793.11	J/mol×K	994.02	Joback Method
cpg	801.77	J/mol×K	1027.89	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=U407623&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