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

Inchi: InChI=1S/C21H21F4NO2/c1-2-3-4-5-6-11-26(20(27)16-9-7-14(22)12-18(16)24)21(28)17-

InchiKey: UVVSQTGPIIGGGP-UHFFFAOYSA-N

Formula: C21H21F4NO2

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

Mol. weight [g/mol]: 395.39

Physical Properties

Property code	Value	Unit	Source
gf	-614.06	kJ/mol	Joback Method
hf	-991.66	kJ/mol	Joback Method
hfus	55.21	kJ/mol	Joback Method
hvap	81.81	kJ/mol	Joback Method
log10ws	-7.42		Crippen Method
logp	5.496		Crippen Method
mcvol	279.430	ml/mol	McGowan Method
pc	1384.02	kPa	Joback Method
rinpol	2311.00		NIST Webbook
rinpol	2311.00		NIST Webbook
tb	870.42	K	Joback Method
tc	1074.64	K	Joback Method
tf	564.04	K	Joback Method
vc	1.097	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	851.67	J/mol×K	870.42	Joback Method
cpg	865.14	J/mol×K	904.46	Joback Method
cpg	877.63	J/mol×K	938.49	Joback Method
cpg	889.19	J/mol×K	972.53	Joback Method
cpg	899.87	J/mol×K	1006.56	Joback Method
cpg	909.74	J/mol×K	1040.60	Joback Method
cpg	918.84	J/mol×K	1074.64	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=U407625&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