Benzamide, 3,4-difluoro-N-(3,4-difluorobenzoyl)-N-hexyl-

Inchi: InChI=1S/C20H19F4NO2/c1-2-3-4-5-10-25(19(26)13-6-8-15(21)17(23)11-13)20(27)14-7-

InchiKey: PBLNHSOMOIFVCB-UHFFFAOYSA-N

Formula: C20H19F4NO2

SMILES: CCCCCCN(C(=O)c1ccc(F)c(F)c1)C(=O)c1ccc(F)c(F)c1

Mol. weight [g/mol]: 381.36

Physical Properties

Property code	Value	Unit	Source
gf	-622.48	kJ/mol	Joback Method
hf	-971.02	kJ/mol	Joback Method
hfus	52.62	kJ/mol	Joback Method
hvap	79.58	kJ/mol	Joback Method
log10ws	-7.00		Crippen Method
logp	5.106		Crippen Method
mcvol	265.340	ml/mol	McGowan Method
pc	1488.44	kPa	Joback Method
rinpol	2182.00		NIST Webbook
rinpol	2182.00		NIST Webbook
tb	847.54	K	Joback Method
tc	1050.91	K	Joback Method
tf	552.77	K	Joback Method
vc	1.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	794.26	J/mol×K	847.54	Joback Method
cpg	807.43	J/mol×K	881.43	Joback Method
cpg	819.64	J/mol×K	915.33	Joback Method
cpg	830.94	J/mol×K	949.22	Joback Method
cpg	841.39	J/mol×K	983.12	Joback Method
cpg	851.03	J/mol×K	1017.01	Joback Method
cpg	859.91	J/mol×K	1050.91	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=U407811&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