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

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

InchiKey: BRGNFFVAPHYPHT-UHFFFAOYSA-N

Formula: C17H13F4NO2

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

Mol. weight [g/mol]: 339.28

Physical Properties

Property code	Value	Unit	Source
gf	-647.74	kJ/mol	Joback Method
hf	-909.10	kJ/mol	Joback Method
hfus	44.85	kJ/mol	Joback Method
hvap	72.90	kJ/mol	Joback Method
log10ws	-5.75		Crippen Method
logp	3.936		Crippen Method
mcvol	223.070	ml/mol	McGowan Method
pc	1883.80	kPa	Joback Method
rinpol	1902.00		NIST Webbook
rinpol	1902.00		NIST Webbook
tb	778.90	K	Joback Method
tc	983.77	K	Joback Method
tf	518.96	K	Joback Method
vc	0.874	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	627.31	J/mol×K	778.90	Joback Method
cpg	639.52	J/mol×K	813.05	Joback Method
cpg	650.82	J/mol×K	847.19	Joback Method
cpg	661.26	J/mol×K	881.34	Joback Method
cpg	670.89	J/mol×K	915.48	Joback Method
cpg	679.75	J/mol×K	949.63	Joback Method
cpg	687.89	J/mol×K	983.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407807&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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