Benzamide, 3,4-difluoro-N-(3,4-difluorobenzoyl)-N-(2-ethylhex

Inchi: InChI=1S/C22H23F4NO2/c1-3-5-6-14(4-2)13-27(21(28)15-7-9-17(23)19(25)11-15)22(29)

InchiKey: AAWBNHVHJXVJRK-UHFFFAOYSA-N

Formula: C22H23F4NO2

SMILES: CCCCC(CC)CN(C(=O)c1ccc(F)c(F)c1)C(=O)c1ccc(F)c(F)c1

Mol. weight [g/mol]: 409.42

Physical Properties

Property code	Value	Unit	Source
gf	-608.08	kJ/mol	Joback Method
hf	-1017.58	kJ/mol	Joback Method
hfus	54.28	kJ/mol	Joback Method
hvap	83.64	kJ/mol	Joback Method
log10ws	-7.60		Crippen Method
logp	5.742		Crippen Method
mcvol	293.520	ml/mol	McGowan Method
pc	1297.66	kPa	Joback Method
rinpol	2261.00		NIST Webbook
rinpol	2261.00		NIST Webbook
tb	892.86	K	Joback Method
tc	1099.92	K	Joback Method
tf	560.31	K	Joback Method
vc	1.147	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	910.37	J/mol×K	892.86	Joback Method
cpg	924.21	J/mol×K	927.37	Joback Method
cpg	937.00	J/mol×K	961.88	Joback Method
cpg	948.82	J/mol×K	996.39	Joback Method
cpg	959.73	J/mol×K	1030.90	Joback Method
cpg	969.78	J/mol×K	1065.41	Joback Method
cpg	979.03	J/mol×K	1099.92	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407812&Units=SI

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