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

Inchi: InChI=1S/C22H23F4NO2/c1-2-3-4-5-6-7-12-27(21(28)15-8-10-17(23)19(25)13-15)22(29)

InchiKey: LFWKBYDTTJMCAU-UHFFFAOYSA-N

Formula: C22H23F4NO2

SMILES: CCCCCCCCN(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	-605.64	kJ/mol	Joback Method
hf	-1012.30	kJ/mol	Joback Method
hfus	57.80	kJ/mol	Joback Method
hvap	84.03	kJ/mol	Joback Method
log10ws	-7.84		Crippen Method
logp	5.886		Crippen Method
mcvol	293.520	ml/mol	McGowan Method
pc	1290.21	kPa	Joback Method
rinpol	2384.00		NIST Webbook
rinpol	2384.00		NIST Webbook
tb	893.30	K	Joback Method
tc	1099.13	K	Joback Method
tf	575.31	K	Joback Method
vc	1.153	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	909.86	J/mol×K	893.30	Joback Method
cpg	923.64	J/mol×K	927.60	Joback Method
cpg	936.41	J/mol×K	961.91	Joback Method
cpg	948.22	J/mol×K	996.21	Joback Method
cpg	959.14	J/mol×K	1030.52	Joback Method
cpg	969.22	J/mol×K	1064.82	Joback Method
cpg	978.53	J/mol×K	1099.13	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=U407814&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