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

Inchi: InChI=1S/C16H11F4NO2/c1-2-21(15(22)9-3-5-11(17)13(19)7-9)16(23)10-4-6-12(18)14(2

InchiKey: XPVBYEASWFYPOD-UHFFFAOYSA-N

Formula: C16H11F4NO2

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

Mol. weight [g/mol]: 325.26

Physical Properties

Property code	Value	Unit	Source
gf	-656.16	kJ/mol	Joback Method
hf	-888.46	kJ/mol	Joback Method
hfus	42.26	kJ/mol	Joback Method
hvap	70.68	kJ/mol	Joback Method
log10ws	-5.33		Crippen Method
logp	3.546		Crippen Method
mcvol	208.980	ml/mol	McGowan Method
pc	2051.17	kPa	Joback Method
rinpol	1824.00		NIST Webbook
rinpol	1824.00		NIST Webbook
tb	756.02	K	Joback Method
tc	962.58	K	Joback Method
tf	507.69	K	Joback Method
vc	0.818	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.65	J/mol×K	756.02	Joback Method
cpg	585.47	J/mol×K	790.45	Joback Method
cpg	596.41	J/mol×K	824.87	Joback Method
cpg	606.51	J/mol×K	859.30	Joback Method
cpg	615.81	J/mol×K	893.73	Joback Method
cpg	624.35	J/mol×K	928.16	Joback Method
cpg	632.18	J/mol×K	962.58	Joback Method

Sources

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=U407806&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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