

3,4-Difluorobenzamide, N,N-dihexyl-

Inchi:	InChI=1S/C19H29F2NO/c1-3-5-7-9-13-22(14-10-8-6-4-2)19(23)16-11-12-17(20)18(21)15
InchiKey:	LHRLGLOHURSFIT-UHFFFAOYSA-N
Formula:	C19H29F2NO
SMILES:	CCCCCN(CCCCC)C(=O)c1ccc(F)c(F)c1
Mol. weight [g/mol]:	325.44

Physical Properties

Property code	Value	Unit	Source
gf	-205.51	kJ/mol	Joback Method
hf	-659.17	kJ/mol	Joback Method
hfus	49.01	kJ/mol	Joback Method
hvap	68.64	kJ/mol	Joback Method
log10ws	-6.46		Crippen Method
logp	5.568		Crippen Method
mvol	269.900	ml/mol	McGowan Method
pc	1303.29	kPa	Joback Method
rinpol	2168.00		NIST Webbook
rinpol	2168.00		NIST Webbook
tb	735.61	K	Joback Method
tc	916.95	K	Joback Method
tf	438.93	K	Joback Method
vc	1.052	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	794.39	J/mol×K	735.61	Joback Method
cpg	811.55	J/mol×K	765.83	Joback Method
cpg	827.78	J/mol×K	796.06	Joback Method
cpg	843.14	J/mol×K	826.28	Joback Method
cpg	857.64	J/mol×K	856.50	Joback Method
cpg	871.34	J/mol×K	886.72	Joback Method
cpg	884.27	J/mol×K	916.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358125&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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