

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

Inchi:	InChI=1S/C23H25F4NO2/c1-2-3-4-5-6-7-8-13-28(22(29)16-9-11-18(24)20(26)14-16)23(3
InchiKey:	JCSZZUFWICOKSV-UHFFFAOYSA-N
Formula:	C23H25F4NO2
SMILES:	CCCCCCCCCN(C(=O)c1ccc(F)c(F)c1)C(=O)c1ccc(F)c(F)c1
Mol. weight [g/mol]:	423.44

Physical Properties

Property code	Value	Unit	Source
gf	-597.22	kJ/mol	Joback Method
hf	-1032.94	kJ/mol	Joback Method
hfus	60.39	kJ/mol	Joback Method
hvap	86.26	kJ/mol	Joback Method
log10ws	-8.26		Crippen Method
logp	6.276		Crippen Method
mcvol	307.610	ml/mol	McGowan Method
pc	1205.63	kPa	Joback Method
rinpol	2486.00		NIST Webbook
rinpol	2486.00		NIST Webbook
tb	916.18	K	Joback Method
tc	1124.44	K	Joback Method
tf	586.58	K	Joback Method
vc	1.210	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	968.78	J/mol×K	916.18	Joback Method
cpg	982.88	J/mol×K	950.89	Joback Method
cpg	995.93	J/mol×K	985.60	Joback Method
cpg	1008.01	J/mol×K	1020.31	Joback Method
cpg	1019.16	J/mol×K	1055.02	Joback Method
cpg	1029.47	J/mol×K	1089.73	Joback Method
cpg	1038.99	J/mol×K	1124.44	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=U407815&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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