

Benzamide, 2,5-difluoro-N-(2,5-difluorobenzoyl)-N-methyl-

Inchi:	InChI=1S/C15H9F4NO2/c1-20(14(21)10-6-8(16)2-4-12(10)18)15(22)11-7-9(17)3-5-13(11)
InchiKey:	MBZDFFHJPGROBS-UHFFFAOYSA-N
Formula:	C15H9F4NO2
SMILES:	CN(C(=O)c1cc(F)ccc1F)C(=O)c1cc(F)ccc1F
Mol. weight [g/mol]:	311.23

Physical Properties

Property code	Value	Unit	Source
gf	-664.58	kJ/mol	Joback Method
hf	-867.82	kJ/mol	Joback Method
hfus	39.67	kJ/mol	Joback Method
hvap	68.45	kJ/mol	Joback Method
log10ws	-4.91		Crippen Method
logp	3.155		Crippen Method
mcvol	194.890	ml/mol	McGowan Method
pc	2241.88	kPa	Joback Method
rinpol	1828.00		NIST Webbook
rinpol	1828.00		NIST Webbook
tb	733.14	K	Joback Method
tc	941.91	K	Joback Method
tf	496.42	K	Joback Method
vc	0.761	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.09	J/molxK	733.14	Joback Method
cpg	532.49	J/molxK	767.94	Joback Method
cpg	543.02	J/molxK	802.73	Joback Method
cpg	552.73	J/molxK	837.53	Joback Method
cpg	561.66	J/molxK	872.32	Joback Method
cpg	569.83	J/molxK	907.12	Joback Method
cpg	577.31	J/molxK	941.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407598&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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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