

2,3,4,5,6-PENTAFLUORO-N-(4-METHOXYPHENYL

Other names:	Benzamide, N-(4-methoxyphenyl)-2,3,4,5,6-pentafluoro-
Inchi:	InChI=1S/C14H8F5NO2/c1-22-7-4-2-6(3-5-7)20-14(21)8-9(15)11(17)13(19)12(18)10(8)1
InchiKey:	HJRCAPVDAKKDQK-UHFFFAOYSA-N
Formula:	C14H8F5NO2
SMILES:	COc1ccc(NC(=O)c2c(F)c(F)c(F)c(F)c2F)cc1
Mol. weight [g/mol]:	317.21

Physical Properties

Property code	Value	Unit	Source
hf	-903.24	kJ/mol	Cheméo Relay (1.0)
hfus	41.05	kJ/mol	Joback Method
hvap	88.89	kJ/mol	Cheméo Relay (1.0)
ie	8.05	eV	Cheméo Relay (1.0)
log10ws	-6.09		Cheméo Relay (1.0)
logp	3.643		Crippen Method
mcvol	186.870	ml/mol	McGowan Method
rinpol	1960.00		NIST Webbook
rinpol	1960.00		NIST Webbook
tb	611.16	K	Cheméo Relay (1.0)
tf	416.64	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.61	J/mol×K	725.77	Joback Method
cpg	509.39	J/mol×K	759.12	Joback Method
cpg	519.43	J/mol×K	792.46	Joback Method
cpg	528.76	J/mol×K	825.81	Joback Method
cpg	537.38	J/mol×K	859.15	Joback Method
cpg	545.29	J/mol×K	892.50	Joback Method
cpg	552.50	J/mol×K	925.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C297149725&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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