

3-Fluoro-5-trifluoromethylbenzamide, N-(4-methoxyphenyl)-

Inchi:	InChI=1S/C15H11F4NO2/c1-22-13-4-2-12(3-5-13)20-14(21)9-6-10(15(17,18)19)8-11(16)
InchiKey:	XZADSQRTUDTTAU-UHFFFAOYSA-N
Formula:	C15H11F4NO2
SMILES:	COc1ccc(NC(=O)c2cc(F)cc(C(F)(F)F)c2)cc1
Mol. weight [g/mol]:	313.25

Physical Properties

Property code	Value	Unit	Source
gf	-649.58	kJ/mol	Joback Method
hf	-898.80	kJ/mol	Joback Method
hfus	34.31	kJ/mol	Joback Method
hvap	66.55	kJ/mol	Joback Method
log10ws	-5.00		Crippen Method
logp	4.105		Crippen Method
mcvol	199.190	ml/mol	McGowan Method
pc	2177.49	kPa	Joback Method
rinpol	2144.00		NIST Webbook
rinpol	2144.00		NIST Webbook
tb	731.21	K	Joback Method
tc	943.31	K	Joback Method
tf	478.81	K	Joback Method
vc	0.779	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	549.46	J/molxK	731.21	Joback Method
cpg	561.77	J/molxK	766.56	Joback Method
cpg	573.12	J/molxK	801.91	Joback Method
cpg	583.55	J/molxK	837.26	Joback Method
cpg	593.12	J/molxK	872.61	Joback Method
cpg	601.87	J/molxK	907.96	Joback Method
cpg	609.86	J/molxK	943.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358148&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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