3-Fluoro-6-trifluoromethylbenzamide, N-(4-methoxyphenyl)-

Inchi: InChI=1S/C15H11F4NO2/c1-22-11-5-3-10(4-6-11)20-14(21)12-8-9(16)2-7-13(12)15(17,1

InchiKey: JFYNNNNNCOFEHT-UHFFFAOYSA-N

Formula: C15H11F4NO2

SMILES: COc1ccc(NC(=O)c2cc(F)ccc2C(F)(F)F)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	2122.00		NIST Webbook
rinpol	2122.00		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/mol×K	731.21	Joback Method
cpg	561.77	J/mol×K	766.56	Joback Method
cpg	573.12	J/mol×K	801.91	Joback Method
cpg	583.55	J/mol×K	837.26	Joback Method
cpg	593.12	J/mol×K	872.61	Joback Method
cpg	601.87	J/mol×K	907.96	Joback Method
cpg	609.86	J/mol×K	943.31	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=U358081&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
hvap:	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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume