4-Fluoro-2-trifluoromethylbenzamide, N-(3-methylphenyl)-

Inchi: InChI=1S/C15H11F4NO/c1-9-3-2-4-11(7-9)20-14(21)12-6-5-10(16)8-13(12)15(17,18)19/h
InchiKey: IFRJXSLFHFAACR-UHFFFAOYSA-N
Formula: C15H11F4NO
SMILES: Cc1cccc(NC(=O)c2ccc(F)cc2C(F)(F)F)c1
Mol. weight [g/mol]: 297.25

Physical Properties

Property code	Value	Unit	Source
gf	-544.58	kJ/mol	Joback Method
hf	-766.58	kJ/mol	Joback Method
hfus	33.12	kJ/mol	Joback Method
hvap	64.14	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	4.405		Crippen Method
mcvol	193.320	ml/mol	McGowan Method
pc	2212.45	kPa	Joback Method
rinpol	1931.00		NIST Webbook
rinpol	1931.00		NIST Webbook
tb	708.79	K	Joback Method
tc	922.89	K	Joback Method
tf	456.58	K	Joback Method
vc	0.761	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.18	J/mol×K	708.79	Joback Method
cpg	536.84	J/mol×K	744.47	Joback Method
cpg	548.52	J/mol×K	780.16	Joback Method
cpg	559.28	J/mol×K	815.84	Joback Method
cpg	569.18	J/mol×K	851.52	Joback Method
cpg	578.30	J/mol×K	887.21	Joback Method
cpg	586.70	J/mol×K	922.89	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=U358089&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

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