p-ACETAMIDOBENZOTRIFLUORIDE

Other names:	4-Trifluoromethylacetanilide
	p-Acetylaminobenzotrifluoride
	Acetamide, N-[4-(trifluoromethyl)phenyl]-
	p-Acetamidobenzotrifluoride
	N-[4-(trifluoromethyl)phenyl]acetamide
Inchi:	InChI=1S/C9H8F3NO/c1-6(14)13-8-4-2-7(3-5-8)9(10,11)12/h2-5H,1H3,(H,13,14)
InchiKey:	DFDHFECLWHHELH-UHFFFAOYSA-N
Formula:	C9H8F3NO
SMILES:	CC(=O)Nc1ccc(C(F)(F)F)cc1
Mol. weight [g/mol]:	203.16

Physical Properties

Property code	Value	Unit	Source
hfus	21.24	kJ/mol	Joback Method
ie	8.86	eV	Cheméo Relay (1.0)
log10ws	-2.36		Cheméo Relay (1.0)
logp	2.664		Crippen Method
mcvol	130.770	ml/mol	McGowan Method
tb	504.87	K	Cheméo Relay (1.0)
tf	388.66	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	306.42	J/mol×K	535.60	Joback Method
cpg	318.10	J/mol×K	569.10	Joback Method
cpg	328.97	J/mol×K	602.61	Joback Method
cpg	339.06	J/mol×K	636.11	Joback Method
cpg	348.43	J/mol×K	669.61	Joback Method
cpg	357.11	J/mol×K	703.12	Joback Method
cpg	365.14	J/mol×K	736.62	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C349973&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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):	

Legend

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