4-AMINOPHENYL TRIFLUOROMETHYL SULPHONE

Inchi: InChI=1S/C7H6F3NO2S/c8-7(9,10)14(12,13)6-3-1-5(11)2-4-6/h1-4H,11H2

InchiKey: GNVFCXUZQGCXPB-UHFFFAOYSA-N

Formula: C7H6F3NO2S

SMILES: Nc1ccc(S(=O)(=O)C(F)(F)F)cc1

Mol. weight [g/mol]: 225.19

Physical Properties

Property code	Value	Unit	Source
hfus	25.94	kJ/mol	Joback Method
ie	8.57	eV	Cheméo Relay (1.0)
log10ws	-2.11		Cheméo Relay (1.0)
logp	1.562		Crippen Method
mcvol	129.110	ml/mol	McGowan Method
tf	384.34	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	289.77	J/mol×K	506.11	Joback Method
cpg	300.87	J/mol×K	539.44	Joback Method
cpg	311.21	J/mol×K	572.78	Joback Method
cpg	320.81	J/mol×K	606.11	Joback Method
cpg	329.70	J/mol×K	639.44	Joback Method
cpg	337.89	J/mol×K	672.77	Joback Method
cpg	345.42	J/mol×K	706.11	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C473278&Units=SI

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
tf:	Normal melting (fusion) point