4-Aminophenyl trifluoromethyl sulfone

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
CAS: 473-27-8

Physical Properties

Property code	Value	Unit	Source
gf	-872.84	kJ/mol	Joback Method
hf	-979.39	kJ/mol	Joback Method
hfus	25.94	kJ/mol	Joback Method
hvap	59.64	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.562		Crippen Method
mcvol	129.110	ml/mol	McGowan Method
pc	4577.74	kPa	Joback Method
tb	506.11	K	Joback Method
tc	706.11	K	Joback Method
tf	333.60	K	Joback Method
vc	0.517	m3/kmol	Joback Method

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C473278&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume