N-Phenyltrifluoromethanesulfonimide

Other names:	N-Phenyl-bis(trifluoromethanesulfonimide)
	N-Phenylbis(trifluoromethanesulphonimide)
	Methanesulfonamide, 1,1,1-trifluoro-N-phenyl-N-[(trifluoromethyl)sulfonyl]-
Inchi:	InChI=1S/C8H5F6NO4S2/c9-7(10,11)20(16,17)15(6-4-2-1-3-5-6)21(18,19)8(12,13)14/h1
InchiKey:	DIOHEXPTUTVCNX-UHFFFAOYSA-N
Formula:	C8H5F6NO4S2
SMILES:	O=S(=O)(N(c1ccccc1)S(=O)(=O)C(F)(F)F)C(F)(F)F
Mol. weight [g/mol]:	357.25
CAS:	37595-74-7

Physical Properties

Property code	Value	Unit	Source
gf	-1860.59	kJ/mol	Joback Method
hf	-2005.25	kJ/mol	Joback Method
hfus	39.95	kJ/mol	Joback Method
hvap	67.50	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	2.192		Crippen Method
mcvol	176.600	ml/mol	McGowan Method
pc	4010.84	kPa	Joback Method
tb	506.28	K	Joback Method
tc	670.88	K	Joback Method
tf	324.31	K	Joback Method
vc	0.732	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.52	J/mol×K	506.28	Joback Method
cpg	428.10	J/mol×K	533.71	Joback Method
cpg	439.84	J/mol×K	561.15	Joback Method
cpg	450.79	J/mol×K	588.58	Joback Method
cpg	460.95	J/mol×K	616.01	Joback Method
cpg	470.37	J/mol×K	643.44	Joback Method

cpg	479.05	J/mol×K	670.88	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C37595747&Units=SI

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