

N-Phenylbis(trifluoromethanesulphonimide)

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

Physical Properties

Property code	Value	Unit	Source
hfus	39.95	kJ/mol	Joback Method
logp	2.192		Crippen Method
mcvol	176.600	ml/mol	McGowan 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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C37595747&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

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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