

p-Tolyl-N-fluoro-N-neopentylsulfonamide

Inchi:	InChI=1S/C12H18FNO2S/c1-10-5-7-11(8-6-10)17(15,16)14(13)9-12(2,3)4/h5-8H,9H2,1-4
InchiKey:	COHNWDUZTLRGOG-UHFFFAOYSA-N
Formula:	C12H18FNO2S
SMILES:	<chem>Cc1ccc(S(=O)(=O)N(F)CC(C)(C)C)cc1</chem>
Mol. weight [g/mol]:	259.34
CAS:	88303-17-7

Physical Properties

Property code	Value	Unit	Source
gf	-396.79	kJ/mol	Joback Method
hf	-656.63	kJ/mol	Joback Method
hfus	30.55	kJ/mol	Joback Method
hvap	63.81	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	2.916		Crippen Method
mcvol	196.020	ml/mol	McGowan Method
pc	2693.00	kPa	Joback Method
tb	561.88	K	Joback Method
tc	755.64	K	Joback Method
tf	337.98	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	478.41	J/molxK	561.88	Joback Method
cpg	495.44	J/molxK	594.17	Joback Method
cpg	511.42	J/molxK	626.47	Joback Method
cpg	526.40	J/molxK	658.76	Joback Method
cpg	540.41	J/molxK	691.05	Joback Method
cpg	553.48	J/molxK	723.35	Joback Method
cpg	565.66	J/molxK	755.64	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	408.00	K	0.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C88303177&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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