p-Tolyl-N-fluoro-N-methylsulfonamide

Inchi: InChI=1S/C8H10FNO2S/c1-7-3-5-8(6-4-7)13(11,12)10(2)9/h3-6H,1-2H3
InchiKey: PGGWSBRXMHAXEG-UHFFFAOYSA-N
Formula: C8H10FNO2S
SMILES: Cc1ccc(S(=O)(=O)N(C)F)cc1
Mol. weight [g/mol]: 203.23
CAS: 88303-12-2

Physical Properties

Property code	Value	Unit	Source
gf	-433.31	kJ/mol	Joback Method
hf	-565.32	kJ/mol	Joback Method
hfus	27.61	kJ/mol	Joback Method
hvap	56.20	kJ/mol	Joback Method
log10ws	-2.04		Crippen Method
logp	1.500		Crippen Method
mcvol	139.660	ml/mol	McGowan Method
pc	4098.62	kPa	Joback Method
tb	473.59	K	Joback Method
tc	665.56	K	Joback Method
tf	290.48	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	289.41	J/mol×K	473.59	Joback Method
cpg	302.57	J/mol×K	505.58	Joback Method
cpg	315.03	J/mol×K	537.58	Joback Method
cpg	326.80	J/mol×K	569.57	Joback Method
cpg	337.90	J/mol×K	601.57	Joback Method
cpg	348.34	J/mol×K	633.56	Joback Method
cpg	358.13	J/mol×K	665.56	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	363.00	K	0.00	NIST Webbook

Sources

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=C88303122&Units=SI
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
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