P-toluenesulfonic acid, 2-fluoroethyl ester

Inchi: InChI=1S/C9H11FO3S/c1-8-2-4-9(5-3-8)14(11,12)13-7-6-10/h2-5H,6-7H2,1H3
InchiKey: XNRDLSNSMTUXBV-UHFFFAOYSA-N
Formula: C9H11FO3S
SMILES: Cc1ccc(S(=O)(=O)OCCF)cc1
Mol. weight [g/mol]: 218.25
CAS: 383-50-6

Physical Properties

Property code	Value	Unit	Source
gf	-640.67	kJ/mol	Joback Method
hf	-785.71	kJ/mol	Joback Method
hfus	28.36	kJ/mol	Joback Method
hvap	58.79	kJ/mol	Joback Method
log10ws	-1.99		Crippen Method
logp	1.670		Crippen Method
mcvol	149.640	ml/mol	McGowan Method
pc	3572.80	kPa	Joback Method
tb	506.45	K	Joback Method
tc	697.28	K	Joback Method
tf	291.51	K	Joback Method
vc	0.594	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.51	J/mol×K	506.45	Joback Method
cpg	337.48	J/mol×K	538.25	Joback Method
cpg	349.85	J/mol×K	570.06	Joback Method
cpg	361.62	J/mol×K	601.86	Joback Method
cpg	372.79	J/mol×K	633.67	Joback Method
cpg	383.35	J/mol×K	665.47	Joback Method
cpg	393.30	J/mol×K	697.28	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C383506&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