Ethanol, 2,2,2-trifluoro-, 4-methylbenzenesulfonate

Other names: Ethanol, 2,2,2-trifluoro-, p-toluenesulfonate
2,2,2-Trifluoroethyl tosylate
2,2,2-Trifluoroethyl p-toluenesulfonate
2,2,2-Trifluoroethyl 4-toluenesulfonate
Trifluoroethanol tosylate
2,2,2-trifluoroethyl p-toluenesulphonate

Inchi: InChI=1S/C9H9F3O3S/c1-7-2-4-8(5-3-7)16(13,14)15-6-9(10,11)12/h2-5H,6H2,1H3

InchiKey: IGKCQDUYZULGBM-UHFFFAOYSA-N

Formula: C9H9F3O3S

SMILES: Cc1ccc(S(=O)(=O)OCC(F)(F)F)cc1

Mol. weight [g/mol]: 254.23

CAS: 433-06-7

Physical Properties

Property code	Value	Unit	Source
gf	-1027.45	kJ/mol	Joback Method
hf	-1186.68	kJ/mol	Joback Method
hfus	27.11	kJ/mol	Joback Method
hvap	55.86	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	2.263		Crippen Method
mcvol	153.180	ml/mol	McGowan Method
pc	3287.81	kPa	Joback Method
tb	501.76	K	Joback Method
tc	685.24	K	Joback Method
tf	295.11	K	Joback Method
vc	0.619	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	344.21	J/mol×K	501.76	Joback Method
cpg	356.91	J/mol×K	532.34	Joback Method
cpg	368.93	J/mol×K	562.92	Joback Method

cpg	380.27	J/mol×K	593.50	Joback Method
cpg	390.95	J/mol×K	624.08	Joback Method
cpg	400.97	J/mol×K	654.66	Joback Method
cpg	410.36	J/mol×K	685.24	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	362.50 ± 0.50	K	0.01	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C433067&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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume