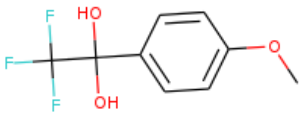
1,1-Ethanediol, 2,2,2-trifluoro-1-(4-methoxyphenyl)-

InChI: InChI=1S/C9H9F3O3/c1-15-7-4-2-6(3-5-7)8(13,14)9(10,11)12/h2-5,13-14H,1H3
InChI Key: OVYVMUARAPGOIN-UHFFFAOYSA-N
Formula: C9H9F3O3
SMILES: COc1ccc(C(O)(O)C(F)(F)F)cc1
Molecular Weight: 222.16
CAS: 110374-82-8



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-829.71	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-1046.54	kJ/mol	Joback Method
$\Delta_{fus} H°$	16.49	kJ/mol	Joback Method
$\Delta_{vap} H°$	69.29	kJ/mol	Joback Method
$logP_{oct/wat}$	1.39		Crippen Method
P_c	3476.55	kPa	Joback Method
T_{boil}	635.11	K	Joback Method
T_c	815.64	K	Joback Method
T_{fus}	380.61	K	Joback Method
V_c	0.52	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	368.60	J/mol×K	635.11	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C9H9F3O3/c1-15-7-4-2-6(3-5-7)8(13,14)9(10,11)12/h2-5,13-14H,1H3

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).
$\Delta_f G°$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f H°_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus} H°$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap} H°$: Enthalpy of vaporization at standard conditions (kJ/mol).
***log*$P_{oct/wat}$**: Octanol/Water partition coefficient .
P_c: Critical Pressure (kPa).
T_{boil}: Normal Boiling Point Temperature (K).
T_c: Critical Temperature (K).
T_{fus}: Normal melting (fusion) point (K).
V_c: Critical Volume (m^3/kg-mol).