Ethylene glycol monosalicylate, bis(trifluoroacetate)

Inchi: InChI=1S/C13H8F6O6/c14-12(15,16)10(21)24-6-5-23-9(20)7-3-1-2-4-8(7)25-11(22)13(17
InchiKey: GWVFRUISTYOCTK-UHFFFAOYSA-N
Formula: C13H8F6O6
SMILES: O=C(OCCOC(=O)C(F)(F)F)c1ccccc1OC(=O)C(F)(F)F
Mol. weight [g/mol]: 374.19

Physical Properties

Property code	Value	Unit	Source
gf	-1703.58	kJ/mol	Joback Method
hf	-2015.15	kJ/mol	Joback Method
hfus	35.09	kJ/mol	Joback Method
hvap	67.44	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	2.417		Crippen Method
mcvol	203.210	ml/mol	McGowan Method
pc	1985.89	kPa	Joback Method
rinpol	1471.00		NIST Webbook
rinpol	1471.00		NIST Webbook
tb	746.53	K	Joback Method
tc	936.07	K	Joback Method
tf	500.07	K	Joback Method
vc	0.814	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	579.26	J/mol×K	746.53	Joback Method
cpg	588.99	J/mol×K	778.12	Joback Method
cpg	597.92	J/mol×K	809.71	Joback Method
cpg	606.09	J/mol×K	841.30	Joback Method
cpg	613.51	J/mol×K	872.89	Joback Method
cpg	620.21	J/mol×K	904.48	Joback Method
cpg	626.22	J/mol×K	936.07	Joback Method

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=U376238&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume