Coniferyl alcohol, bis(trifluoroacetate)

Inchi: InChI=1S/C14H10F6O5/c1-23-10-7-8(3-2-6-24-11(21)13(15,16)17)4-5-9(10)25-12(22)14
InchiKey: YFJAKLUPKYORII-NSCUHMNNSA-N
Formula: C14H10F6O5
SMILES: COc1cc(C=CCOC(=O)C(F)(F)F)ccc1OC(=O)C(F)(F)F
Mol. weight [g/mol]: 372.22

Physical Properties

Property code	Value	Unit	Source
gf	-1495.65	kJ/mol	Joback Method
hf	-1817.46	kJ/mol	Joback Method
hfus	35.89	kJ/mol	Joback Method
hvap	63.54	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	3.282		Crippen Method
mcvol	211.430	ml/mol	McGowan Method
pc	1786.37	kPa	Joback Method
rinpol	1614.00		NIST Webbook
rinpol	1614.00		NIST Webbook
tb	724.68	K	Joback Method
tc	912.27	K	Joback Method
tf	468.85	K	Joback Method
vc	0.844	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.77	J/mol×K	724.68	Joback Method
cpg	604.64	J/mol×K	755.95	Joback Method
cpg	614.74	J/mol×K	787.21	Joback Method
cpg	624.09	J/mol×K	818.48	Joback Method
cpg	632.73	J/mol×K	849.74	Joback Method
cpg	640.69	J/mol×K	881.01	Joback Method
cpg	648.00	J/mol×K	912.27	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375741&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume