1-Phenoxypropan-2-yl trifluoroacetate

Other names: 2-Phenoxy-1-methylethyl trifluoroacetate
Phenoxyisopropanyl trifluoroacetate
Inchi: InChI=1S/C11H11F3O3/c1-8(17-10(15)11(12,13)14)7-16-9-5-3-2-4-6-9/h2-6,8H,7H2,1H3
InchiKey: IMTYBMZPGKODON-UHFFFAOYSA-N
Formula: C11H11F3O3
SMILES: CC(COc1ccccc1)OC(=O)C(F)(F)F
Mol. weight [g/mol]: 248.20

Physical Properties

Property code	Value	Unit	Source
gf	-768.80	kJ/mol	Joback Method
hf	-1013.22	kJ/mol	Joback Method
hfus	20.57	kJ/mol	Joback Method
hvap	49.79	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.559		Crippen Method
mcvol	160.710	ml/mol	McGowan Method
pc	2445.89	kPa	Joback Method
rinpol	1254.00		NIST Webbook
tb	570.61	K	Joback Method
tc	764.95	K	Joback Method
tf	323.73	K	Joback Method
vc	0.623	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.60	J/mol×K	570.61	Joback Method
cpg	412.87	J/mol×K	603.00	Joback Method
cpg	425.33	J/mol×K	635.39	Joback Method
cpg	437.02	J/mol×K	667.78	Joback Method
cpg	447.96	J/mol×K	700.17	Joback Method
cpg	458.16	J/mol×K	732.56	Joback Method
cpg	467.66	J/mol×K	764.95	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=U372959&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