3-Phenoxypropyl 2,2,2-trifluoroacetate

Inchi: InChI=1S/C11H11F3O3/c12-11(13,14)10(15)17-8-4-7-16-9-5-2-1-3-6-9/h1-3,5-6H,4,7-8H
InchiKey: NKHOOSPTQZZMDE-UHFFFAOYSA-N
Formula: C11H11F3O3
SMILES: O=C(OCCCOc1ccccc1)C(F)(F)F
Mol. weight [g/mol]: 248.20

Physical Properties

Property code	Value	Unit	Source
gf	-766.36	kJ/mol	Joback Method
hf	-1007.94	kJ/mol	Joback Method
hfus	24.09	kJ/mol	Joback Method
hvap	50.17	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	2.561		Crippen Method
mcvol	160.710	ml/mol	McGowan Method
pc	2426.65	kPa	Joback Method
rinpol	1330.00		NIST Webbook
rinpol	1330.00		NIST Webbook
tb	571.05	K	Joback Method
tc	761.63	K	Joback Method
tf	338.73	K	Joback Method
vc	0.628	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.22	J/mol×K	571.05	Joback Method
cpg	412.18	J/mol×K	602.81	Joback Method
cpg	424.37	J/mol×K	634.58	Joback Method
cpg	435.82	J/mol×K	666.34	Joback Method
cpg	446.56	J/mol×K	698.10	Joback Method
cpg	456.60	J/mol×K	729.86	Joback Method
cpg	465.96	J/mol×K	761.63	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=U378330&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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