Propanoic acid, pentafluoro-, 1-phenylethyl ester

Other names: 1-Phenylethanol, pentafluoropropionate
Inchi: InChI=1S/C11H9F5O2/c1-7(8-5-3-2-4-6-8)18-9(17)10(12,13)11(14,15)16/h2-7H,1H3
InchiKey: GQZAFSYCSMSOJI-UHFFFAOYSA-N
Formula: C11H9F5O2
SMILES: CC(OC(=O)C(F)(F)C(F)(F)F)c1ccccc1
Mol. weight [g/mol]: 268.18
CAS: 55702-47-1

Physical Properties

Property code	Value	Unit	Source
gf	-1050.58	kJ/mol	Joback Method
hf	-1281.97	kJ/mol	Joback Method
hfus	18.12	kJ/mol	Joback Method
hvap	44.45	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.488		Crippen Method
mcvol	158.380	ml/mol	McGowan Method
pc	2320.31	kPa	Joback Method
rinpol	1041.00		NIST Webbook
tb	543.50	K	Joback Method
tc	732.21	K	Joback Method
tf	305.10	K	Joback Method
vc	0.629	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.54	J/mol×K	543.50	Joback Method
cpg	407.75	J/mol×K	574.95	Joback Method
cpg	420.04	J/mol×K	606.40	Joback Method
cpg	431.45	J/mol×K	637.85	Joback Method
cpg	442.02	J/mol×K	669.30	Joback Method
cpg	451.81	J/mol×K	700.76	Joback Method
cpg	460.86	J/mol×K	732.21	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55702471&Units=SI

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