3-Phenoxypropyl 2,2,3,3,3-pentafluoropropanoate

Inchi: InChI=1S/C12H11F5O3/c13-11(14,12(15,16)17)10(18)20-8-4-7-19-9-5-2-1-3-6-9/h1-3,5-

InchiKey: VCSXYEUPLBDCRJ-UHFFFAOYSA-N

Formula: C12H11F5O3

SMILES: O=C(OCCCOc1ccccc1)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 298.21

Physical Properties

Property code	Value	Unit	Source
gf	-1144.72	kJ/mol	Joback Method
hf	-1429.55	kJ/mol	Joback Method
hfus	25.42	kJ/mol	Joback Method
hvap	49.47	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	3.196		Crippen Method
mcvol	178.340	ml/mol	McGowan Method
pc	2071.76	kPa	Joback Method
rinpol	1344.00		NIST Webbook
tb	589.24	K	Joback Method
tc	771.35	K	Joback Method
tf	353.60	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	467.06	J/mol×K	589.24	Joback Method
cpg	480.11	J/mol×K	619.59	Joback Method
cpg	492.32	J/mol×K	649.94	Joback Method
cpg	503.74	J/mol×K	680.30	Joback Method
cpg	514.38	J/mol×K	710.65	Joback Method
cpg	524.30	J/mol×K	741.00	Joback Method
cpg	533.52	J/mol×K	771.35	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=U378346&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