Pentafluoropropanoic acid, 4-benzyloxyphenyl ester

Inchi: InChI=1S/C16H11F5O3/c17-15(18,16(19,20)21)14(22)24-13-8-6-12(7-9-13)23-10-11-4-2

InchiKey: ZOQSBSNUTWFGEI-UHFFFAOYSA-N

Formula: C16H11F5O3

SMILES: O=C(Oc1ccc(OCc2ccccc2)cc1)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 346.25

Physical Properties

Property code	Value	Unit	Source
gf	-1008.26	kJ/mol	Joback Method
hf	-1287.05	kJ/mol	Joback Method
hfus	29.44	kJ/mol	Joback Method
hvap	61.31	kJ/mol	Joback Method
log10ws	-5.41		Crippen Method
logp	4.369		Crippen Method
mcvol	210.940	ml/mol	McGowan Method
pc	1949.23	kPa	Joback Method
rinpol	1720.00		NIST Webbook
tb	712.42	K	Joback Method
tc	920.20	K	Joback Method
tf	437.62	K	Joback Method
vc	0.826	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	589.04	J/mol×K	712.42	Joback Method
cpg	602.09	J/mol×K	747.05	Joback Method
cpg	614.08	J/mol×K	781.68	Joback Method
cpg	625.05	J/mol×K	816.31	Joback Method
cpg	635.08	J/mol×K	850.94	Joback Method
cpg	644.22	J/mol×K	885.57	Joback Method
cpg	652.56	J/mol×K	920.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308008&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