Benzene, pentafluoropropionyl

Inchi: InChI=1S/C9H5F5O/c10-8(11,9(12,13)14)7(15)6-4-2-1-3-5-6/h1-5H
InchiKey: VUBUXALTYMBEQO-UHFFFAOYSA-N
Formula: C9H5F5O
SMILES: O=C(c1ccccc1)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 224.13

Physical Properties

Property code	Value	Unit	Source
gf	-959.98	kJ/mol	Joback Method
hf	-1103.19	kJ/mol	Joback Method
hfus	15.28	kJ/mol	Joback Method
hvap	37.97	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	3.067		Crippen Method
mcvol	124.330	ml/mol	McGowan Method
pc	2844.44	kPa	Joback Method
rinpol	906.00		NIST Webbook
rinpol	906.00		NIST Webbook
tb	475.76	K	Joback Method
tc	666.13	K	Joback Method
tf	275.33	K	Joback Method
vc	0.505	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.17	J/mol×K	475.76	Joback Method
cpg	293.22	J/mol×K	507.49	Joback Method
cpg	304.33	J/mol×K	539.22	Joback Method
cpg	314.53	J/mol×K	570.95	Joback Method
cpg	323.90	J/mol×K	602.67	Joback Method
cpg	332.49	J/mol×K	634.40	Joback Method
cpg	340.34	J/mol×K	666.13	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=R515236&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