2-(4-Fluorophenyl)-1,1,1,3,3,3-hexafluoro-2-propa

Inchi: InChI=1S/C9H5F7O/c10-6-3-1-5(2-4-6)7(17,8(11,12)13)9(14,15)16/h1-4,17H
InchiKey: VFFCPASLKRVTCD-UHFFFAOYSA-N
Formula: C9H5F7O
SMILES: OC(c1ccc(F)cc1)(C(F)(F)F)C(F)(F)F
Mol. weight [g/mol]: 262.12
CAS: 2402-74-6

Physical Properties

Property code	Value	Unit	Source
gf	-1364.29	kJ/mol	Joback Method
hf	-1555.28	kJ/mol	Joback Method
hfus	16.12	kJ/mol	Joback Method
hvap	45.64	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	3.138		Crippen Method
mcvol	132.170	ml/mol	McGowan Method
pc	2679.08	kPa	Joback Method
tb	514.36	K	Joback Method
tc	681.54	K	Joback Method
tf	302.34	K	Joback Method
vc	0.543	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.88	J/mol×K	514.36	Joback Method
cpg	345.04	J/mol×K	542.22	Joback Method
cpg	354.41	J/mol×K	570.09	Joback Method
cpg	363.06	J/mol×K	597.95	Joback Method
cpg	371.02	J/mol×K	625.81	Joback Method
cpg	378.33	J/mol×K	653.67	Joback Method
cpg	385.06	J/mol×K	681.54	Joback Method

Sources

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=C2402746&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume