2,3,4,5-Tetrafluorobenzyl alcohol, n-pentyl ether

Inchi: InChI=1S/C12H14F4O/c1-2-3-4-5-17-7-8-6-9(13)11(15)12(16)10(8)14/h6H,2-5,7H2,1H3
InchiKey: VKKIGJPVAQGFOE-UHFFFAOYSA-N
Formula: C12H14F4O
SMILES: CCCCCOCc1cc(F)c(F)c(F)c1F
Mol. weight [g/mol]: 250.23

Physical Properties

Property code	Value	Unit	Source
gf	-760.19	kJ/mol	Joback Method
hf	-1017.02	kJ/mol	Joback Method
hfus	32.83	kJ/mol	Joback Method
hvap	46.37	kJ/mol	Joback Method
log10ws	-4.86		Crippen Method
logp	3.950		Crippen Method
mcvol	169.130	ml/mol	McGowan Method
pc	1896.95	kPa	Joback Method
rinpol	1320.00		NIST Webbook
rinpol	1320.00		NIST Webbook
tb	540.06	K	Joback Method
tc	708.26	K	Joback Method
tf	326.09	K	Joback Method
vc	0.690	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	405.93	J/mol×K	540.06	Joback Method
cpg	418.54	J/mol×K	568.09	Joback Method
cpg	430.68	J/mol×K	596.13	Joback Method
cpg	442.34	J/mol×K	624.16	Joback Method
cpg	453.53	J/mol×K	652.19	Joback Method
cpg	464.25	J/mol×K	680.23	Joback Method
cpg	474.51	J/mol×K	708.26	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=U375292&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