2,3,4,5-Tetrafluorobenzyl alcohol, 3-methylbutyl ether

Inchi: InChI=1S/C12H14F4O/c1-7(2)3-4-17-6-8-5-9(13)11(15)12(16)10(8)14/h5,7H,3-4,6H2,1-2

InchiKey: NDQHQKMKEVKBPF-UHFFFAOYSA-N

Formula: C12H14F4O

SMILES: CC(C)CCOCc1cc(F)c(F)c(F)c1F

Mol. weight [g/mol]: 250.23

Physical Properties

Property code	Value	Unit	Source
gf	-762.63	kJ/mol	Joback Method
hf	-1022.30	kJ/mol	Joback Method
hfus	29.31	kJ/mol	Joback Method
hvap	45.98	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	3.806		Crippen Method
mcvol	169.130	ml/mol	McGowan Method
pc	1910.24	kPa	Joback Method
rinpol	1281.00		NIST Webbook
rinpol	1281.00		NIST Webbook
tb	539.62	K	Joback Method
tc	710.90	K	Joback Method
tf	311.09	K	Joback Method
vc	0.683	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.23	J/mol×K	539.62	Joback Method
cpg	419.13	J/mol×K	568.17	Joback Method
cpg	431.53	J/mol×K	596.71	Joback Method
cpg	443.43	J/mol×K	625.26	Joback Method
cpg	454.84	J/mol×K	653.81	Joback Method
cpg	465.76	J/mol×K	682.36	Joback Method
cpg	476.18	J/mol×K	710.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375293&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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