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

Inchi: InChI=1S/C11H12F4O/c1-2-3-4-16-6-7-5-8(12)10(14)11(15)9(7)13/h5H,2-4,6H2,1H3
InchiKey: XYPXCYPFCFHOHF-UHFFFAOYSA-N
Formula: C11H12F4O
SMILES: CCCCOCc1cc(F)c(F)c(F)c1F
Mol. weight [g/mol]: 236.21

Physical Properties

Property code	Value	Unit	Source
gf	-768.61	kJ/mol	Joback Method
hf	-996.38	kJ/mol	Joback Method
hfus	30.24	kJ/mol	Joback Method
hvap	44.15	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	3.560		Crippen Method
mcvol	155.040	ml/mol	McGowan Method
pc	2066.12	kPa	Joback Method
rinpol	1224.00		NIST Webbook
tb	517.18	K	Joback Method
tc	686.50	K	Joback Method
tf	314.82	K	Joback Method
vc	0.633	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	359.96	J/mol×K	517.18	Joback Method
cpg	371.72	J/mol×K	545.40	Joback Method
cpg	383.04	J/mol×K	573.62	Joback Method
cpg	393.94	J/mol×K	601.84	Joback Method
cpg	404.41	J/mol×K	630.06	Joback Method
cpg	414.45	J/mol×K	658.28	Joback Method
cpg	424.07	J/mol×K	686.50	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375296&Units=SI

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