

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

Inchi:	InChI=1S/C10H10F4O/c1-2-3-15-5-6-4-7(11)9(13)10(14)8(6)12/h4H,2-3,5H2,1H3
InchiKey:	XKUQFOLZKXWKPT-UHFFFAOYSA-N
Formula:	C10H10F4O
SMILES:	CCCOc1cc(F)c(F)c(F)c1F
Mol. weight [g/mol]:	222.18

Physical Properties

Property code	Value	Unit	Source
gf	-777.03	kJ/mol	Joback Method
hf	-975.74	kJ/mol	Joback Method
hfus	27.65	kJ/mol	Joback Method
hvap	41.92	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	3.170		Crippen Method
mcvol	140.950	ml/mol	McGowan Method
pc	2258.96	kPa	Joback Method
rinpol	1129.00		NIST Webbook
tb	494.30	K	Joback Method
tc	664.85	K	Joback Method
tf	303.55	K	Joback Method
vc	0.578	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.92	J/molxK	494.30	Joback Method
cpg	326.72	J/molxK	522.73	Joback Method
cpg	337.14	J/molxK	551.15	Joback Method
cpg	347.18	J/molxK	579.58	Joback Method
cpg	356.84	J/molxK	608.00	Joback Method
cpg	366.12	J/molxK	636.43	Joback Method
cpg	375.02	J/molxK	664.85	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=U375297&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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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

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