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

Inchi: InChI=1S/C12H15F3O/c1-8(2)3-4-16-7-9-5-11(14)12(15)6-10(9)13/h5-6,8H,3-4,7H2,1-2H

InchiKey: YQCOABNSMKBGON-UHFFFAOYSA-N

Formula: C12H15F3O

SMILES: CC(C)CCOCc1cc(F)c(F)cc1F

Mol. weight [g/mol]: 232.24

Physical Properties

Property code	Value	Unit	Source
gf	-558.19	kJ/mol	Joback Method
hf	-814.72	kJ/mol	Joback Method
hfus	26.61	kJ/mol	Joback Method
hvap	46.14	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	3.667		Crippen Method
mcvol	167.360	ml/mol	McGowan Method
pc	2014.51	kPa	Joback Method
rinpol	1290.00		NIST Webbook
rinpol	1290.00		NIST Webbook
tb	535.37	K	Joback Method
tc	713.35	K	Joback Method
tf	297.98	K	Joback Method
vc	0.665	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.86	J/mol×K	535.37	Joback Method
cpg	411.62	J/mol×K	565.03	Joback Method
cpg	424.80	J/mol×K	594.70	Joback Method
cpg	437.42	J/mol×K	624.36	Joback Method
cpg	449.47	J/mol×K	654.02	Joback Method
cpg	460.97	J/mol×K	683.69	Joback Method
cpg	471.93	J/mol×K	713.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375254&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

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