2,4,5-Trifluorobenzyl alcohol, tert.-butyl ether

Inchi: InChI=1S/C11H13F3O/c1-11(2,3)15-6-7-4-9(13)10(14)5-8(7)12/h4-5H,6H2,1-3H3
InchiKey: LHFMJBWBEOFNGJ-UHFFFAOYSA-N
Formula: C11H13F3O
SMILES: CC(C)(C)OCc1cc(F)c(F)cc1F
Mol. weight [g/mol]: 218.22

Physical Properties

Property code	Value	Unit	Source
gf	-561.33	kJ/mol	Joback Method
hf	-797.55	kJ/mol	Joback Method
hfus	20.13	kJ/mol	Joback Method
hvap	43.01	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	3.419		Crippen Method
mcvol	153.270	ml/mol	McGowan Method
pc	2222.89	kPa	Joback Method
rinpol	1154.00		NIST Webbook
tb	509.70	K	Joback Method
tc	696.14	K	Joback Method
tf	304.13	K	Joback Method
vc	0.605	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	354.65	J/mol×K	509.70	Joback Method
cpg	368.18	J/mol×K	540.77	Joback Method
cpg	381.03	J/mol×K	571.85	Joback Method
cpg	393.24	J/mol×K	602.92	Joback Method
cpg	404.82	J/mol×K	633.99	Joback Method
cpg	415.79	J/mol×K	665.06	Joback Method
cpg	426.17	J/mol×K	696.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375253&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