3,4,5-Trifluorobenzyl alcohol, n-butyl ether

Inchi: InChI=1S/C11H13F3O/c1-2-3-4-15-7-8-5-9(12)11(14)10(13)6-8/h5-6H,2-4,7H2,1H3
InchiKey: RQGHHBLIJPHAFF-UHFFFAOYSA-N
Formula: C11H13F3O
SMILES: CCCCOCc1cc(F)c(F)c(F)c1
Mol. weight [g/mol]: 218.22

Physical Properties

Property code	Value	Unit	Source
gf	-564.17	kJ/mol	Joback Method
hf	-788.80	kJ/mol	Joback Method
hfus	27.55	kJ/mol	Joback Method
hvap	44.30	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.421		Crippen Method
mcvol	153.270	ml/mol	McGowan Method
pc	2183.60	kPa	Joback Method
rinpol	1257.00		NIST Webbook
rinpol	1257.00		NIST Webbook
tb	512.93	K	Joback Method
tc	689.06	K	Joback Method
tf	301.71	K	Joback Method
vc	0.616	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.51	J/mol×K	512.93	Joback Method
cpg	364.10	J/mol×K	542.28	Joback Method
cpg	376.20	J/mol×K	571.64	Joback Method
cpg	387.79	J/mol×K	600.99	Joback Method
cpg	398.90	J/mol×K	630.35	Joback Method
cpg	409.52	J/mol×K	659.70	Joback Method
cpg	419.67	J/mol×K	689.06	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375247&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