3,4,5-Trifluorobenzyl alcohol, isopropyl ether

Inchi: InChI=1S/C10H11F3O/c1-6(2)14-5-7-3-8(11)10(13)9(12)4-7/h3-4,6H,5H2,1-2H3
InchiKey: WRNOMEZWKWCWDZ-UHFFFAOYSA-N
Formula: C10H11F3O
SMILES: CC(C)OCc1cc(F)c(F)c(F)c1
Mol. weight [g/mol]: 204.19

Physical Properties

Property code	Value	Unit	Source
gf	-575.03	kJ/mol	Joback Method
hf	-773.44	kJ/mol	Joback Method
hfus	21.43	kJ/mol	Joback Method
hvap	41.69	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	3.029		Crippen Method
mcvol	139.180	ml/mol	McGowan Method
pc	2412.37	kPa	Joback Method
rinpol	1120.00		NIST Webbook
tb	489.61	K	Joback Method
tc	671.06	K	Joback Method
tf	275.44	K	Joback Method
vc	0.553	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.58	J/mol×K	489.61	Joback Method
cpg	319.54	J/mol×K	519.85	Joback Method
cpg	331.02	J/mol×K	550.09	Joback Method
cpg	342.03	J/mol×K	580.34	Joback Method
cpg	352.58	J/mol×K	610.58	Joback Method
cpg	362.65	J/mol×K	640.82	Joback Method
cpg	372.26	J/mol×K	671.06	Joback Method

Sources

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=U375249&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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