2,4,5-Trifluorobenzyl alcohol

Inchi: InChI=1S/C7H5F3O/c8-5-2-7(10)6(9)1-4(5)3-11/h1-2,11H,3H2
InchiKey: NRXZCCOHXZFHBV-UHFFFAOYSA-N
Formula: C7H5F3O
SMILES: OCc1cc(F)c(F)cc1F
Mol. weight [g/mol]: 162.11
CAS: 144284-25-3

Physical Properties

Property code	Value	Unit	Source
gf	-629.67	kJ/mol	Joback Method
hf	-726.25	kJ/mol	Joback Method
hfus	20.09	kJ/mol	Joback Method
hvap	49.67	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	1.596		Crippen Method
mcvol	96.910	ml/mol	McGowan Method
pc	3686.49	kPa	Joback Method
tb	491.17	K	Joback Method
tc	666.50	K	Joback Method
tf	295.22	K	Joback Method
vc	0.393	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	206.76	J/mol×K	491.17	Joback Method
cpg	214.04	J/mol×K	520.39	Joback Method
cpg	221.00	J/mol×K	549.61	Joback Method
cpg	227.63	J/mol×K	578.83	Joback Method
cpg	233.96	J/mol×K	608.05	Joback Method
cpg	239.99	J/mol×K	637.28	Joback Method
cpg	245.72	J/mol×K	666.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C144284253&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume