2,6-Dichlorobenzyl alcohol, trifluoroacetate

Inchi: InChI=1S/C9H5Cl2F3O2/c10-6-2-1-3-7(11)5(6)4-16-8(15)9(12,13)14/h1-3H,4H2
InchiKey: PSVXTGHHBXSOHR-UHFFFAOYSA-N
Formula: C9H5Cl2F3O2
SMILES: O=C(OCc1c(Cl)cccc1Cl)C(F)(F)F
Mol. weight [g/mol]: 273.04

Physical Properties

Property code	Value	Unit	Source
gf	-721.32	kJ/mol	Joback Method
hf	-888.86	kJ/mol	Joback Method
hfus	25.34	kJ/mol	Joback Method
hvap	53.41	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	3.599		Crippen Method
mcvol	151.140	ml/mol	McGowan Method
pc	2698.60	kPa	Joback Method
rinpol	1310.00		NIST Webbook
rinpol	1310.00		NIST Webbook
tb	587.69	K	Joback Method
tc	796.07	K	Joback Method
tf	378.84	K	Joback Method
vc	0.597	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	331.64	J/mol×K	587.69	Joback Method
cpg	341.06	J/mol×K	622.42	Joback Method
cpg	349.80	J/mol×K	657.15	Joback Method
cpg	357.89	J/mol×K	691.88	Joback Method
cpg	365.36	J/mol×K	726.61	Joback Method
cpg	372.24	J/mol×K	761.34	Joback Method
cpg	378.55	J/mol×K	796.07	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376099&Units=SI

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