2,6-Dichlorobenzyl alcohol, heptafluorobutyrate

Inchi: InChI=1S/C11H5Cl2F7O2/c12-6-2-1-3-7(13)5(6)4-22-8(21)9(14,15)10(16,17)11(18,19)20

InchiKey: ZVDPTEHWNOCIEA-UHFFFAOYSA-N

Formula: C11H5Cl2F7O2

SMILES: O=C(OCc1c(Cl)cccc1Cl)C(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 373.05

Physical Properties

Property code	Value	Unit	Source
gf	-1478.04	kJ/mol	Joback Method
hf	-1732.08	kJ/mol	Joback Method
hfus	28.01	kJ/mol	Joback Method
hvap	52.00	kJ/mol	Joback Method
log10ws	-5.55		Crippen Method
logp	4.870		Crippen Method
mcvol	186.400	ml/mol	McGowan Method
pc	1959.60	kPa	Joback Method
rinpol	1355.00		NIST Webbook
rinpol	1355.00		NIST Webbook
tb	624.07	K	Joback Method
tc	813.33	K	Joback Method
tf	408.58	K	Joback Method
vc	0.758	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.57	J/mol×K	624.07	Joback Method
cpg	474.38	J/mol×K	655.61	Joback Method
cpg	483.37	J/mol×K	687.16	Joback Method
cpg	491.58	J/mol×K	718.70	Joback Method
cpg	499.09	J/mol×K	750.24	Joback Method
cpg	505.95	J/mol×K	781.79	Joback Method
cpg	512.21	J/mol×K	813.33	Joback Method

Sources

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=U376097&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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