2,4-Dichlorobenzyl alcohol, pentafluoropropionate

Inchi: InChI=1S/C10H5Cl2F5O2/c11-6-2-1-5(7(12)3-6)4-19-8(18)9(13,14)10(15,16)17/h1-3H,4H

InchiKey: LHRQFFGDGMRILG-UHFFFAOYSA-N

Formula: C10H5Cl2F5O2

SMILES: O=C(OCc1ccc(Cl)cc1Cl)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 323.04

Physical Properties

Property code	Value	Unit	Source
gf	-1099.68	kJ/mol	Joback Method
hf	-1310.47	kJ/mol	Joback Method
hfus	26.67	kJ/mol	Joback Method
hvap	52.70	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.234		Crippen Method
mcvol	168.770	ml/mol	McGowan Method
pc	2284.95	kPa	Joback Method
rinpol	1341.00		NIST Webbook
rinpol	1341.00		NIST Webbook
tb	605.88	K	Joback Method
tc	803.98	K	Joback Method
tf	393.71	K	Joback Method
vc	0.677	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.59	J/mol×K	605.88	Joback Method
cpg	407.29	J/mol×K	638.90	Joback Method
cpg	416.22	J/mol×K	671.91	Joback Method
cpg	424.43	J/mol×K	704.93	Joback Method
cpg	431.96	J/mol×K	737.94	Joback Method
cpg	438.85	J/mol×K	770.96	Joback Method
cpg	445.16	J/mol×K	803.98	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=U376086&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