4-Chlorobenzyl alcohol, pentafluoropropionate

Inchi: InChI=1S/C10H6ClF5O2/c11-7-3-1-6(2-4-7)5-18-8(17)9(12,13)10(14,15)16/h1-4H,5H2
InchiKey: YNOUQZHJUWTECY-UHFFFAOYSA-N
Formula: C10H6ClF5O2
SMILES: O=C(OCc1ccc(Cl)cc1)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 288.60
CAS: 958997-71-2

Physical Properties

Property code	Value	Unit	Source
gf	-1078.12	kJ/mol	Joback Method
hf	-1283.26	kJ/mol	Joback Method
hfus	22.86	kJ/mol	Joback Method
hvap	47.66	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	3.581		Crippen Method
mcvol	156.530	ml/mol	McGowan Method
pc	2402.92	kPa	Joback Method
rinpol	1193.00		NIST Webbook
rinpol	1193.00		NIST Webbook
tb	563.47	K	Joback Method
tc	756.35	K	Joback Method
tf	351.27	K	Joback Method
vc	0.628	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	374.47	J/mol×K	563.47	Joback Method
cpg	385.42	J/mol×K	595.62	Joback Method
cpg	395.55	J/mol×K	627.76	Joback Method
cpg	404.90	J/mol×K	659.91	Joback Method
cpg	413.52	J/mol×K	692.06	Joback Method
cpg	421.46	J/mol×K	724.21	Joback Method
cpg	428.75	J/mol×K	756.35	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=C958997712&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