2,6-Dichlorophenol, heptafluorobutyrate

Inchi: InChI=1S/C10H3Cl2F7O2/c11-4-2-1-3-5(12)6(4)21-7(20)8(13,14)9(15,16)10(17,18)19/h1
InchiKey: FAHSDAJNAQGEMS-UHFFFAOYSA-N
Formula: C10H3Cl2F7O2
SMILES: O=C(Oc1c(Cl)cccc1Cl)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 359.02

Physical Properties

Property code	Value	Unit	Source
gf	-1486.46	kJ/mol	Joback Method
hf	-1711.44	kJ/mol	Joback Method
hfus	25.42	kJ/mol	Joback Method
hvap	49.77	kJ/mol	Joback Method
log10ws	-5.28		Crippen Method
logp	4.732		Crippen Method
mcvol	172.310	ml/mol	McGowan Method
pc	2137.41	kPa	Joback Method
rinpol	1227.00		NIST Webbook
tb	601.19	K	Joback Method
tc	792.57	K	Joback Method
tf	397.31	K	Joback Method
vc	0.703	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	417.78	J/mol×K	601.19	Joback Method
cpg	427.01	J/mol×K	633.09	Joback Method
cpg	435.43	J/mol×K	664.98	Joback Method
cpg	443.07	J/mol×K	696.88	Joback Method
cpg	450.02	J/mol×K	728.78	Joback Method
cpg	456.31	J/mol×K	760.67	Joback Method
cpg	462.01	J/mol×K	792.57	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=U374858&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