2,3,5-Trichlorophenol, O-heptafluorobutyryl-

Inchi: InChI=1S/C10H2Cl3F7O2/c11-3-1-4(12)6(13)5(2-3)22-7(21)8(14,15)9(16,17)10(18,19)20
InchiKey: CDIXTPKRHJLRNO-UHFFFAOYSA-N
Formula: C10H2Cl3F7O2
SMILES: O=C(Oc1cc(Cl)cc(Cl)c1Cl)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 393.47

Physical Properties

Property code	Value	Unit	Source
gf	-1508.02	kJ/mol	Joback Method
hf	-1738.65	kJ/mol	Joback Method
hfus	29.23	kJ/mol	Joback Method
hvap	54.82	kJ/mol	Joback Method
log10ws	-5.97		Crippen Method
logp	5.385		Crippen Method
mcvol	184.550	ml/mol	McGowan Method
pc	2038.23	kPa	Joback Method
rinpol	1328.00		NIST Webbook
tb	643.60	K	Joback Method
tc	839.91	K	Joback Method
tf	439.75	K	Joback Method
vc	0.751	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.23	J/mol×K	643.60	Joback Method
cpg	446.19	J/mol×K	676.32	Joback Method
cpg	453.41	J/mol×K	709.04	Joback Method
cpg	459.93	J/mol×K	741.76	Joback Method
cpg	465.81	J/mol×K	774.47	Joback Method
cpg	471.12	J/mol×K	807.19	Joback Method
cpg	475.92	J/mol×K	839.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374271&Units=SI
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

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