1,4-Dioxane-2,3-diol, chlorodifluoroacetate, pentafluoropropionate

Inchi: InChI=1S/C9H6ClF7O6/c10-8(13,14)6(19)23-4-3(20-1-2-21-4)22-5(18)7(11,12)9(15,16)1

InchiKey: YONGQMUYEMGJTO-UHFFFAOYSA-N

Formula: C9H6ClF7O6

SMILES: O=C(OC1OCCOC1OC(=O)C(F)(F)C(F)(F)F)C(F)(F)Cl

Mol. weight [g/mol]: 378.58

Physical Properties

Property code	Value	Unit	Source
gf	-1965.52	kJ/mol	Joback Method
hf	-2363.47	kJ/mol	Joback Method
hfus	37.02	kJ/mol	Joback Method
hvap	57.86	kJ/mol	Joback Method
log10ws	-2.54		Crippen Method
logp	1.801		Crippen Method
mcvol	178.060	ml/mol	McGowan Method
pc	2202.08	kPa	Joback Method
rinpol	1145.00		NIST Webbook
rinpol	1145.00		NIST Webbook
tb	649.31	K	Joback Method
tc	836.13	K	Joback Method
tf	433.10	K	Joback Method
vc	0.704	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	511.28	J/mol×K	649.31	Joback Method
cpg	522.37	J/mol×K	680.45	Joback Method
cpg	532.59	J/mol×K	711.58	Joback Method
cpg	541.95	J/mol×K	742.72	Joback Method
cpg	550.51	J/mol×K	773.86	Joback Method
cpg	558.29	J/mol×K	804.99	Joback Method
cpg	565.33	J/mol×K	836.13	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=U375757&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