2-Butene-1,4-diol, O-chlorodifluoroacetate-O'-pentafluoropropionate

Inchi: InChI=1S/C9H6ClF7O4/c10-8(13,14)6(19)21-4-2-1-3-20-5(18)7(11,12)9(15,16)17/h1-2H,

InchiKey: RCVPIFMRZNHUFO-OWOJBTEDSA-N

Formula: C9H6ClF7O4

SMILES: O=C(OCC=CCOC(=O)C(F)(F)C(F)(F)F)C(F)(F)Cl

Mol. weight [g/mol]: 346.58

Physical Properties

Property code	Value	Unit	Source
gf	-1729.80	kJ/mol	Joback Method
hf	-2016.23	kJ/mol	Joback Method
hfus	28.36	kJ/mol	Joback Method
hvap	48.68	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	2.658		Crippen Method
mcvol	172.880	ml/mol	McGowan Method
pc	2005.50	kPa	Joback Method
rinpol	1099.00		NIST Webbook
rinpol	1099.00		NIST Webbook
tb	584.69	K	Joback Method
tc	753.07	K	Joback Method
tf	371.74	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.71	J/mol×K	584.69	Joback Method
cpg	452.18	J/mol×K	612.75	Joback Method
cpg	460.97	J/mol×K	640.82	Joback Method
cpg	469.13	J/mol×K	668.88	Joback Method
cpg	476.69	J/mol×K	696.95	Joback Method
cpg	483.69	J/mol×K	725.01	Joback Method
cpg	490.16	J/mol×K	753.07	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=U375876&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