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

Inchi: InChI=1S/C10H6ClF9O4/c11-8(14,15)6(22)24-4-2-1-3-23-5(21)7(12,13)9(16,17)10(18,19

InchiKey: YNSJANUQLBTQFW-OWOJBTEDSA-N

Formula: C10H6ClF9O4

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

Mol. weight [g/mol]: 396.59

Physical Properties

Property code	Value	Unit	Source
gf	-2108.16	kJ/mol	Joback Method
hf	-2437.84	kJ/mol	Joback Method
hfus	29.69	kJ/mol	Joback Method
hvap	47.97	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	3.293		Crippen Method
mcvol	190.510	ml/mol	McGowan Method
pc	1736.11	kPa	Joback Method
rinpol	1140.00		NIST Webbook
rinpol	1140.00		NIST Webbook
tb	602.88	K	Joback Method
tc	765.87	K	Joback Method
tf	386.61	K	Joback Method
vc	0.790	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	509.75	J/mol×K	602.88	Joback Method
cpg	519.40	J/mol×K	630.04	Joback Method
cpg	528.33	J/mol×K	657.21	Joback Method
cpg	536.58	J/mol×K	684.37	Joback Method
cpg	544.19	J/mol×K	711.54	Joback Method
cpg	551.21	J/mol×K	738.70	Joback Method
cpg	557.68	J/mol×K	765.87	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375875&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