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

Inchi: InChI=1S/C8H6ClF5O4/c9-7(10,11)5(15)17-3-1-2-4-18-6(16)8(12,13)14/h1-2H,3-4H2/b2-

InchiKey: BZTKEZPVZFFBRS-OWOJBTEDSA-N

Formula: C8H6ClF5O4

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

Mol. weight [g/mol]: 296.58

Physical Properties

Property code	Value	Unit	Source
gf	-1351.44	kJ/mol	Joback Method
hf	-1594.62	kJ/mol	Joback Method
hfus	27.02	kJ/mol	Joback Method
hvap	49.38	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	2.023		Crippen Method
mcvol	155.250	ml/mol	McGowan Method
pc	2342.82	kPa	Joback Method
rinpol	1248.00		NIST Webbook
rinpol	1248.00		NIST Webbook
tb	566.50	K	Joback Method
tc	741.54	K	Joback Method
tf	356.87	K	Joback Method
vc	0.628	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.79	J/mol×K	566.50	Joback Method
cpg	385.94	J/mol×K	595.67	Joback Method
cpg	394.48	J/mol×K	624.85	Joback Method
cpg	402.45	J/mol×K	654.02	Joback Method
cpg	409.88	J/mol×K	683.19	Joback Method
cpg	416.79	J/mol×K	712.37	Joback Method
cpg	423.21	J/mol×K	741.54	Joback Method

Sources

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=U375877&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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