Diethylene glycol, bis(chlorodifluoroacetate)

Inchi: InChI=1S/C8H8Cl2F4O5/c9-7(11,12)5(15)18-3-1-17-2-4-19-6(16)8(10,13)14/h1-4H2
InchiKey: GQKXNODITGSJSC-UHFFFAOYSA-N
Formula: C8H8Cl2F4O5
SMILES: O=C(OCCOCCOC(=O)C(F)(F)Cl)C(F)(F)Cl
Mol. weight [g/mol]: 331.05

Physical Properties

Property code	Value	Unit	Source
gf	-1353.78	kJ/mol	Joback Method
hf	-1663.69	kJ/mol	Joback Method
hfus	29.12	kJ/mol	Joback Method
hvap	57.03	kJ/mol	Joback Method
log10ws	-1.91		Crippen Method
logp	1.753		Crippen Method
mcvol	175.890	ml/mol	McGowan Method
pc	2210.37	kPa	Joback Method
rinpol	1332.00		NIST Webbook
rinpol	1332.00		NIST Webbook
tb	622.92	K	Joback Method
tc	802.60	K	Joback Method
tf	413.51	K	Joback Method
vc	0.698	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.63	J/mol×K	622.92	Joback Method
cpg	444.88	J/mol×K	652.87	Joback Method
cpg	453.55	J/mol×K	682.81	Joback Method
cpg	461.65	J/mol×K	712.76	Joback Method
cpg	469.20	J/mol×K	742.71	Joback Method
cpg	476.22	J/mol×K	772.66	Joback Method
cpg	482.71	J/mol×K	802.60	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=U375791&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