Ethylene glycol, chlorodifluoroacetate, heptafluorobutyrate

Inchi: InChI=1S/C8H4ClF9O4/c9-6(12,13)4(20)22-2-1-21-3(19)5(10,11)7(14,15)8(16,17)18/h1-

InchiKey: GXVRUNRZBFSWHZ-UHFFFAOYSA-N

Formula: C8H4ClF9O4

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

Mol. weight [g/mol]: 370.55

Physical Properties

Property code	Value	Unit	Source
gf	-2205.22	kJ/mol	Joback Method
hf	-2513.78	kJ/mol	Joback Method
hfus	24.31	kJ/mol	Joback Method
hvap	43.56	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	2.737		Crippen Method
mcvol	166.630	ml/mol	McGowan Method
pc	1957.87	kPa	Joback Method
rinpol	981.00		NIST Webbook
tb	552.96	K	Joback Method
tc	711.07	K	Joback Method
tf	369.15	K	Joback Method
vc	0.699	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.69	J/mol×K	552.96	Joback Method
cpg	445.89	J/mol×K	579.31	Joback Method
cpg	454.42	J/mol×K	605.66	Joback Method
cpg	462.31	J/mol×K	632.02	Joback Method
cpg	469.60	J/mol×K	658.37	Joback Method
cpg	476.33	J/mol×K	684.72	Joback Method
cpg	482.52	J/mol×K	711.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375914&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