Diethylene glycol, chlorodifluoroacetate, trifluoroacetate

Inchi: InChI=1S/C8H8ClF5O5/c9-7(10,11)5(15)18-3-1-17-2-4-19-6(16)8(12,13)14/h1-4H2
InchiKey: AZONZZQZSGPSMD-UHFFFAOYSA-N
Formula: C8H8ClF5O5
SMILES: O=C(OCCOCCOC(=O)C(F)(F)Cl)C(F)(F)F
Mol. weight [g/mol]: 314.59

Physical Properties

Property code	Value	Unit	Source
gf	-1536.66	kJ/mol	Joback Method
hf	-1844.06	kJ/mol	Joback Method
hfus	28.01	kJ/mol	Joback Method
hvap	51.83	kJ/mol	Joback Method
log10ws	-1.61		Crippen Method
logp	1.483		Crippen Method
mcvol	165.420	ml/mol	McGowan Method
pc	2193.84	kPa	Joback Method
rinpol	1170.00		NIST Webbook
tb	584.76	K	Joback Method
tc	753.20	K	Joback Method
tf	384.18	K	Joback Method
vc	0.666	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.79	J/mol×K	584.76	Joback Method
cpg	429.36	J/mol×K	612.83	Joback Method
cpg	438.41	J/mol×K	640.91	Joback Method
cpg	446.93	J/mol×K	668.98	Joback Method
cpg	454.95	J/mol×K	697.05	Joback Method
cpg	462.47	J/mol×K	725.13	Joback Method
cpg	469.50	J/mol×K	753.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375793&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