Diethylene glycol, chlorodifluoroacetate, pentafluoropropionate

Inchi: InChI=1S/C9H8ClF7O5/c10-8(13,14)6(19)22-4-2-20-1-3-21-5(18)7(11,12)9(15,16)17/h1-

InchiKey: QNIMPPMDJVEBDG-UHFFFAOYSA-N

Formula: C9H8ClF7O5

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

Mol. weight [g/mol]: 364.60

Physical Properties

Property code	Value	Unit	Source
gf	-1915.02	kJ/mol	Joback Method
hf	-2265.67	kJ/mol	Joback Method
hfus	29.34	kJ/mol	Joback Method
hvap	51.13	kJ/mol	Joback Method
log10ws	-2.34		Crippen Method
logp	2.119		Crippen Method
mcvol	183.050	ml/mol	McGowan Method
pc	1887.08	kPa	Joback Method
rinpol	1185.00		NIST Webbook
rinpol	1185.00		NIST Webbook
tb	602.95	K	Joback Method
tc	765.99	K	Joback Method
tf	399.05	K	Joback Method
vc	0.748	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	486.88	J/mol×K	602.95	Joback Method
cpg	496.73	J/mol×K	630.12	Joback Method
cpg	505.97	J/mol×K	657.30	Joback Method
cpg	514.62	J/mol×K	684.47	Joback Method
cpg	522.71	J/mol×K	711.64	Joback Method
cpg	530.26	J/mol×K	738.81	Joback Method
cpg	537.29	J/mol×K	765.99	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=U375792&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