

Diethylene glycol monoethyl ether, chlorodifluoroacetate

Inchi:	InChI=1S/C8H13ClF2O4/c1-2-13-3-4-14-5-6-15-7(12)8(9,10)11/h2-6H2,1H3
InchiKey:	CECOVAGVDQHUX-UHFFFAOYSA-N
Formula:	C8H13ClF2O4
SMILES:	CCOCCOCCOC(=O)C(F)(F)Cl
Mol. weight [g/mol]:	246.64

Physical Properties

Property code	Value	Unit	Source
gf	-826.15	kJ/mol	Joback Method
hf	-1134.40	kJ/mol	Joback Method
hfus	24.58	kJ/mol	Joback Method
hvap	48.83	kJ/mol	Joback Method
log10ws	-1.17		Crippen Method
logp	1.414		Crippen Method
mcvol	158.540	ml/mol	McGowan Method
pc	2306.95	kPa	Joback Method
rinpol	1182.00		NIST Webbook
tb	536.31	K	Joback Method
tc	709.18	K	Joback Method
tf	330.06	K	Joback Method
vc	0.618	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.31	J/mol×K	536.31	Joback Method
cpg	386.59	J/mol×K	565.12	Joback Method
cpg	397.39	J/mol×K	593.93	Joback Method
cpg	407.74	J/mol×K	622.74	Joback Method
cpg	417.61	J/mol×K	651.56	Joback Method
cpg	427.03	J/mol×K	680.37	Joback Method
cpg	435.98	J/mol×K	709.18	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=U376250&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

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