Ethylene glycol, chlorodifluoroacetate, trifluoroacetate

Inchi: InChI=1S/C6H4ClF5O4/c7-5(8,9)3(13)15-1-2-16-4(14)6(10,11)12/h1-2H2
InchiKey: WEGKAQXNHGDHHE-UHFFFAOYSA-N
Formula: C6H4ClF5O4
SMILES: O=C(OCCOC(=O)C(F)(F)Cl)C(F)(F)F
Mol. weight [g/mol]: 270.54

Physical Properties

Property code	Value	Unit	Source
gf	-1448.50	kJ/mol	Joback Method
hf	-1670.56	kJ/mol	Joback Method
hfus	21.64	kJ/mol	Joback Method
hvap	44.97	kJ/mol	Joback Method
log10ws	-1.68		Crippen Method
logp	1.467		Crippen Method
mcvol	131.370	ml/mol	McGowan Method
pc	2695.80	kPa	Joback Method
rinpol	911.00		NIST Webbook
rinpol	911.00		NIST Webbook
tb	516.58	K	Joback Method
tc	687.47	K	Joback Method
tf	339.41	K	Joback Method
vc	0.536	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.78	J/mol×K	516.58	Joback Method
cpg	316.90	J/mol×K	545.06	Joback Method
cpg	324.54	J/mol×K	573.54	Joback Method
cpg	331.69	J/mol×K	602.02	Joback Method
cpg	338.38	J/mol×K	630.51	Joback Method
cpg	344.63	J/mol×K	658.99	Joback Method
cpg	350.45	J/mol×K	687.47	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=U375916&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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