

Ethylene glycol, chlorodifluoroacetate, pentafluoropropionate

Inchi: InChI=1S/C7H4ClF7O4/c8-6(11,12)4(17)19-2-1-18-3(16)5(9,10)7(13,14)15/h1-2H2
InchiKey: QIOIGSLMAMANKA-UHFFFAOYSA-N
Formula: C7H4ClF7O4
SMILES: O=C(OCCOC(=O)C(F)(F)C(F)(F)F)C(F)(F)Cl
Mol. weight [g/mol]: 320.55

Physical Properties

Property code	Value	Unit	Source
gf	-1826.86	kJ/mol	Joback Method
hf	-2092.17	kJ/mol	Joback Method
hfus	22.98	kJ/mol	Joback Method
hvap	44.27	kJ/mol	Joback Method
log10ws	-2.42		Crippen Method
logp	2.102		Crippen Method
mcvol	149.000	ml/mol	McGowan Method
pc	2282.77	kPa	Joback Method
rinpol	939.00		NIST Webbook
rinpol	939.00		NIST Webbook
tb	534.77	K	Joback Method
tc	698.71	K	Joback Method
tf	354.28	K	Joback Method
vc	0.618	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.98	J/mol×K	534.77	Joback Method
cpg	380.74	J/mol×K	562.09	Joback Method
cpg	388.91	J/mol×K	589.42	Joback Method
cpg	396.51	J/mol×K	616.74	Joback Method
cpg	403.56	J/mol×K	644.06	Joback Method
cpg	410.10	J/mol×K	671.39	Joback Method
cpg	416.15	J/mol×K	698.71	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375915&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

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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