

Diethylene glycol methyl ether, chlorodifluoroacetate

Inchi: InChI=1S/C7H11ClF2O4/c1-12-2-3-13-4-5-14-6(11)7(8,9)10/h2-5H2,1H3
InchiKey: XAINHTLJHRKGSO-UHFFFAOYSA-N
Formula: C7H11ClF2O4
SMILES: COCCOCCOC(=O)C(F)(F)Cl
Mol. weight [g/mol]: 232.61

Physical Properties

Property code	Value	Unit	Source
gf	-834.57	kJ/mol	Joback Method
hf	-1113.76	kJ/mol	Joback Method
hfus	21.99	kJ/mol	Joback Method
hvap	46.61	kJ/mol	Joback Method
log10ws	-0.75		Crippen Method
logp	1.024		Crippen Method
mcvol	144.450	ml/mol	McGowan Method
pc	2535.37	kPa	Joback Method
rinpol	1122.00		NIST Webbook
tb	513.43	K	Joback Method
tc	687.71	K	Joback Method
tf	318.79	K	Joback Method
vc	0.561	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	330.89	J/mol×K	513.43	Joback Method
cpg	341.25	J/mol×K	542.48	Joback Method
cpg	351.19	J/mol×K	571.52	Joback Method
cpg	360.71	J/mol×K	600.57	Joback Method
cpg	369.82	J/mol×K	629.62	Joback Method
cpg	378.52	J/mol×K	658.66	Joback Method
cpg	386.79	J/mol×K	687.71	Joback Method

Sources

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=U376236&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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