

Diethylene glycol monoethyl ether, chlorodifluoroacetate

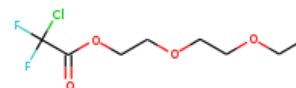
InChI: InChI=1S/C8H13ClF2O4/c1-2-13-3-4-14-5-6-15-7(12)8(9,10)11/h2-6H2,1H3

InChI Key: CECO VAGVDQHUX-UHFFFAOYSA-N

Formula: C₈H₁₃ClF₂O₄

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

Molecular Weight: 246.64



Physical Properties

| Property | Value | Unit | Source |
|---------------------------------|----------|------------------------|----------------|
| $\Delta_f G^\circ$ | -826.15 | kJ/mol | Joback Method |
| $\Delta_f H^\circ_{\text{gas}}$ | -1134.40 | kJ/mol | Joback Method |
| $\Delta_{\text{fus}} H^\circ$ | 24.58 | kJ/mol | Joback Method |
| $\Delta_{\text{vap}} H^\circ$ | 48.83 | kJ/mol | Joback Method |
| $\log P_{\text{oct/wat}}$ | 1.414 | | Crippen Method |
| P_c | 2306.95 | kPa | Joback Method |
| T_{boil} | 536.31 | K | Joback Method |
| T_c | 709.18 | K | Joback Method |
| T_{fus} | 330.06 | K | Joback Method |
| V_c | 0.618 | m ³ /kg-mol | Joback Method |

Temperature Dependent Properties

| Property | Value | Unit | Temperature (K) | Source |
|--------------------|--------|---------|-----------------|---------------|
| $C_{p,\text{gas}}$ | 375.31 | J/mol×K | 536.31 | Joback Method |

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C8H13ClF2O4/c1-2-13-3-4-14-5-6-15-7\(12\)8\(9,10\)11/h2-6H2,1H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C8H13ClF2O4/c1-2-13-3-4-14-5-6-15-7(12)8(9,10)11/h2-6H2,1H3)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$C_{p, gas}$: Ideal gas heat capacity (J/mol×K).

$\Delta_f G^\circ$: Standard Gibbs free energy of formation (kJ/mol).

$\Delta_f H^\circ_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{fus} H^\circ$: Enthalpy of fusion at standard conditions (kJ/mol).

$\Delta_{vap} H^\circ$: Enthalpy of vaporization at standard conditions (kJ/mol).

$logP_{oct/wat}$: Octanol/Water partition coefficient .

P_c : Critical Pressure (kPa).

T_{boil} : Normal Boiling Point Temperature (K).

T_c : Critical Temperature (K).

T_{fus} : Normal melting (fusion) point (K).

V_c : Critical Volume (m³/kg-mol).

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