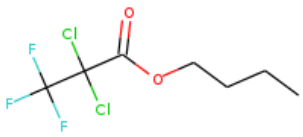
Propionic acid, 2,2-dichloro-3,3,3-trifluoro-, n-butyl ester

InChI:
InChI=1S/C7H9Cl2F3O2/c1-2-3-4-14-5(13)6(8,9)7(10,11)12/h2-4H2,1H3
InChI Key: UEOPJKJKJBWUIQ-UHFFFAOYSA-N
Formula: C7H9Cl2F3O2
SMILES: CCCCOC(=O)C(Cl)(Cl)C(F)(F)F
Molecular Weight: 253.05
CAS: 309-23-9



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-828.47	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-1069.92	kJ/mol	Joback Method
$\Delta_{fus} H°$	19.48	kJ/mol	Joback Method
$\Delta_{vap} H°$	44.06	kJ/mol	Joback Method
$logP_{oct/wat}$	3.07		Crippen Method
P_c	2462.92	kPa	Joback Method
T_{boil}	502.06	K	Joback Method
T_c	684.78	K	Joback Method
T_{fus}	307.26	K	Joback Method
V_c	0.58	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	322.47	J/mol×K	502.06	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C7H9Cl2F3O2/c1-2-3-4-14-5(13)6(8,9)7(10,11)12/h2-4H2,1H3

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
$\mathbf{\Delta_f G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\mathbf{\Delta_f H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\mathbf{\Delta_{fus} H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\mathbf{\Delta_{vap} H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\mathbf{\mathit{log}P_{oct/wat}}$: Octanol/Water partition coefficient .
$\mathbf{P_c}$: Critical Pressure (kPa).
$\mathbf{T_{boil}}$: Normal Boiling Point Temperature (K).
$\mathbf{T_c}$: Critical Temperature (K).
$\mathbf{T_{fus}}$: Normal melting (fusion) point (K).
$\mathbf{V_c}$: Critical Volume (m^3/kg-mol).