4-Hexen-1-ol, (4e)-, heptafluorobutyrate

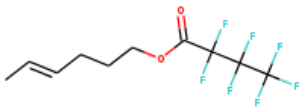
InChI: InChI=1S/C10H11F7O2/c1-2-3-4-5-6-19-7(18)8(11,12)9(13,14)10(15,16)17/h2-3H,4-6H2,1H3/b3-2+

InChI Key: WNMALWPOFDNDKZ-NSCUHMNNSA-N

Formula: C10H11F7O2

SMILES: CC=CCCCOC(=O)C(F)(F)C(F)(F)C(F)(F)F

Molecular Weight: 296.18



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-1475.53	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-1776.33	kJ/mol	Joback Method
$\Delta_{fus} H°$	23.96	kJ/mol	Joback Method
$\Delta_{vap} H°$	37.36	kJ/mol	Joback Method
$logP_{oct/wat}$	3.72		Crippen Method
P_c	1829.41	kPa	Joback Method
T_{boil}	493.85	K	Joback Method
T_c	647.78	K	Joback Method
T_{fus}	280.93	K	Joback Method
V_c	0.69	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	417.08	J/mol×K	493.85	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C10H11F7O2/c1-2-3-4-5-6-19-7(18)8(11,12)9(13,14)10(15,16)17/h2-3H,4-6H2,1H3/b3-2+

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

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).
$\Delta_f G°$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f H°_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus} H°$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap} H°$: Enthalpy of vaporization at standard conditions (kJ/mol).
$log P_{oct/wat}$: 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 (m^3/kg-mol).