

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

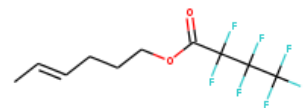
InChI: InChI=1S/C10H11F7O2/c1-2-3-4-5-6-19-7(18)8(11,12)9(13,14)10(15,16)17/h2-3H,4-6H2,1H3/b3-2+

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
$\Delta_f G^\circ$	-1475.53	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-1776.33	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	23.96	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	37.36	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	3.719		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	0.693	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	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+](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/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).

$\log P_{oct/wat}$: 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 (m³/kg-mol).

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