

Heptafluorobutyric acid, undecyl ester

Other names: Undecyl heptafluorobutyrate.

InChI: InChI=1S/C15H23F7O2/c1-2-3-4-5-6-7-8-9-10-11-24-12(23)13(16,17)14(18,19)15(20,21)22/h2-11H2,1H3

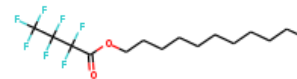
InChI Key: BAMRUWAHGSFKKX-UHFFFAOYSA-N

Formula: C15H23F7O2

SMILES: CCCCCCCCCCOC(=O)C(F)(F)C(F)(F)C(F)(F)F

Molecular Weight: 368.33

CAS: 959103-74-3



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-1513.65	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-1996.75	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	36.71	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	48.53	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	5.89		Crippen Method
P_c	1214.05	kPa	Joback Method
T_{boil}	604.09	K	Joback Method
T_c	754.43	K	Joback Method
T_{fus}	342.36	K	Joback Method
V_c	0.99	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	684.52	J/mol×K	604.09	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C15H23F7O2/c1-2-3-4-5-6-7-8-9-10-11-24-12\(23\)13\(16,17\)14\(18,19\)15\(20,21\)22/h2-11H2,1H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C15H23F7O2/c1-2-3-4-5-6-7-8-9-10-11-24-12(23)13(16,17)14(18,19)15(20,21)22/h2-11H2,1H3)

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).

$\log P_{oct/wat}$: 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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