

Mandelic acid, 3-hydroxy, DCTFA-acetate

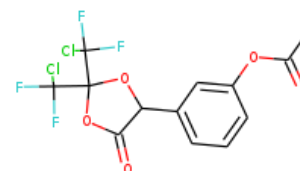
InChI: InChI=1S/C13H8Cl2F4O5/c1-6(20)22-8-4-2-3-7(5-8)9-10(21)24-11(23-9,12(14,16)17)13(15,18)19/h2-5,9H,1H3

InChI Key: NFIKAKAFHSSFLW-UHFFFAOYSA-N

Formula: C13H8Cl2F4O5

SMILES: CC(=O)Oc1cccc(C2OC(C(F)(F)Cl)(C(F)(F)Cl)OC2=O)c1

Molecular Weight: 391.10



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-1141.46	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-1511.13	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	35.93	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	71.60	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	3.59		Crippen Method
P_c	2244.00	kPa	Joback Method
T_{boil}	802.84	K	Joback Method
T_c	1038.43	K	Joback Method
T_{fus}	566.33	K	Joback Method
V_c	0.81	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	603.07	J/mol×K	802.84	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C13H8Cl2F4O5/c1-6\(20\)22-8-4-2-3-7\(5-8\)9-10\(21\)24-11\(23-9,12\(14,16\)17\)13\(15,18\)19/h2-5,9H,1H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C13H8Cl2F4O5/c1-6(20)22-8-4-2-3-7(5-8)9-10(21)24-11(23-9,12(14,16)17)13(15,18)19/h2-5,9H,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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