

Succinic acid, 3-methylbut-2-en-1-yl 1-bromo-3,3,3-trifluoroprop-2-yl ester

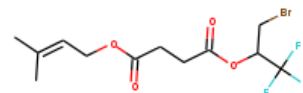
InChI: InChI=1S/C12H16BrF3O4/c1-8(2)5-6-19-10(17)3-4-11(18)20-9(7-13)12(14,15)16/h5,9H,3-4,6-7H2,1-2H3

InChI Key: BKGAOIMVEOTFFV-UHFFFAOYSA-N

Formula: C12H16BrF3O4

SMILES: CC(C)=CCOC(=O)CCC(=O)OC(CBr)C(F)(F)F

Molecular Weight: 361.15



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-915.72	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-1249.21	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	34.89	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	62.96	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	3.15		Crippen Method
P_c	1957.87	kPa	Joback Method
T_{boil}	690.88	K	Joback Method
T_c	878.70	K	Joback Method
T_{fus}	399.27	K	Joback Method
V_c	0.84	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	563.20	J/mol×K	690.88	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H16BrF3O4/c1-8\(2\)5-6-19-10\(17\)3-4-11\(18\)20-9\(7-13\)12\(14,15\)16/h5,9H,3-4,6-7H2,1-2H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H16BrF3O4/c1-8(2)5-6-19-10(17)3-4-11(18)20-9(7-13)12(14,15)16/h5,9H,3-4,6-7H2,1-2H3)

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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