

2,6-Difluorobenzoic acid, pent-2-en-4-ynyl ester

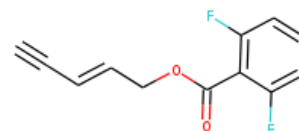
InChI: InChI=1S/C12H8F2O2/c1-2-3-4-8-16-12(15)11-9(13)6-5-7-10(11)14/h1,3-7H,8H2/b4-3+

InChI Key: PXUHUXMKEIVSBN-ONEGZZNKSA-N

Formula: C₁₂H₈F₂O₂

SMILES: C#CC=CCOC(=O)c1c(F)cccc1F

Molecular Weight: 222.19



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-176.94	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-305.32	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	32.22	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	53.24	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	2.31		Crippen Method
P_c	2732.56	kPa	Joback Method
T_{boil}	579.71	K	Joback Method
T_c	790.32	K	Joback Method
T_{fus}	391.69	K	Joback Method
V_c	0.60	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	350.06	J/mol×K	579.71	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H8F2O2/c1-2-3-4-8-16-12\(15\)11-9\(13\)6-5-7-10\(11\)14/h1,3-7H,8H2/b4-3+](http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H8F2O2/c1-2-3-4-8-16-12(15)11-9(13)6-5-7-10(11)14/h1,3-7H,8H2/b4-3+)

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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