

.BETA.-alanine, n-(3-trifluoromethylbenzoyl)-, nonyl ester

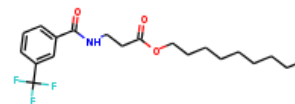
InChI: InChI=1S/C20H28F3NO3/c1-2-3-4-5-6-7-8-14-27-18(25)12-13-24-19(26)16-10-9-11-17(15-16)20(21,22)23/h9-11,15H,2-8,12-14H2,1H3,(H,24,26)

InChI Key: AWBYTQJZYZZDCU-UHFFFAOYSA-N

Formula: C20H28F3NO3

SMILES: CCCCCCCCCOC(=O)CCNC(=O)c1cccc(C(F)(F)F)c1

Molecular Weight: 387.44



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-634.74	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-1132.06	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	52.52	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	81.64	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	5.119		Crippen Method
P_c	1261.06	kPa	Joback Method
T_{boil}	863.57	K	Joback Method
T_c	1061.28	K	Joback Method
T_{fus}	533.04	K	Joback Method
V_c	1.155	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	930.66	J/mol×K	863.57	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C20H28F3NO3/c1-2-3-4-5-6-7-8-14-27-18\(25\)12-13-24-19\(26\)16-10-9-11-17\(15-16\)20\(21,22\)23/h9-11,15H,2-8,12-14H2,1H3,\(H,24,26\)](http://webbook.nist.gov/cgi/inchi/InChI=1S/C20H28F3NO3/c1-2-3-4-5-6-7-8-14-27-18(25)12-13-24-19(26)16-10-9-11-17(15-16)20(21,22)23/h9-11,15H,2-8,12-14H2,1H3,(H,24,26))

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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