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

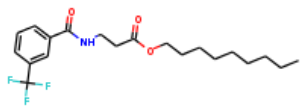
InChI: InChI=1S/C20H28F3NO3/c1-2-3-4-5-6-7-8-14-27-18(25)12-13-24-19(26)16-10-9-11-17(15-16)20(21,22)23/h9-11,15H,2-8,12-14H2,1H3,(H,24,26)

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
$\Delta_f G°$	-634.74	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-1132.06	kJ/mol	Joback Method
$\Delta_{fus} H°$	52.52	kJ/mol	Joback Method
$\Delta_{vap} H°$	81.64	kJ/mol	Joback Method
$logP_{oct/wat}$	5.12		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	1.16	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	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)

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).
$\Delta_f G°$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f H°_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus} H°$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap} H°$: 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 (m^3/kg-mol).