Trans-cinnamamide, n,n-dibutyl-3-trifluoromethyl-

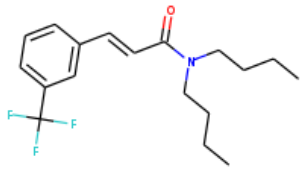
InChI: InChI=1S/C18H24F3NO/c1-3-5-12-22(13-6-4-2)17(23)11-10-15-8-7-9-16(14-15)18(19,20)21/h7-11,14H,3-6,12-13H2,1-2H3/b11-10+

InChI Key: JMRJMFJETQQTKT-ZHACJKMWSA-N

Formula: C18H24F3NO

SMILES: CCCCN(CCCC)C(=O)C=Cc1cccc(C(F)(F)F)c1

Molecular Weight: 327.38



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-316.05	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-714.70	kJ/mol	Joback Method
$\Delta_{fus} H°$	42.68	kJ/mol	Joback Method
$\Delta_{vap} H°$	63.60	kJ/mol	Joback Method
$logP_{oct/wat}$	5.15		Crippen Method
P_c	1442.44	kPa	Joback Method
T_{boil}	707.95	K	Joback Method
T_c	894.34	K	Joback Method
T_{fus}	413.07	K	Joback Method
V_c	0.98	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	724.60	J/mol×K	707.95	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C18H24F3NO/c1-3-5-12-22(13-6-4-2)17(23)11-10-15-8-7-9-16(14-15)18(19,20)21/h7-11,14H,3-6,12-13H2,1-2H3/b11-10+

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

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
$\mathbf{\Delta_f G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\mathbf{\Delta_f H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\mathbf{\Delta_{fus} H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\mathbf{\Delta_{vap} H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\mathbf{\mathit{log}P_{oct/wat}}$: Octanol/Water partition coefficient .
$\mathbf{P_c}$: Critical Pressure (kPa).
$\mathbf{T_{boil}}$: Normal Boiling Point Temperature (K).
$\mathbf{T_c}$: Critical Temperature (K).
$\mathbf{T_{fus}}$: Normal melting (fusion) point (K).
$\mathbf{V_c}$: Critical Volume (m^3/kg-mol).