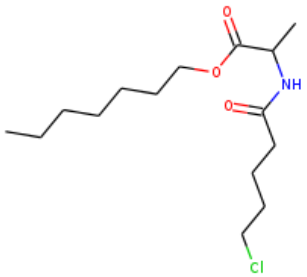
D-alanine, n-(5-chlorovaleryl)-, heptyl ester

InChI: InChI=1S/C15H28ClNO3/c1-3-4-5-6-9-12-20-15(19)13(2)17-14(18)10-7-8-11-16/h13H,3-12H2,1-2H3,(H,17,18)
InChI Key: KOFVZRFXZTVRON-UHFFFAOYSA-N
Formula: C15H28ClNO3
SMILES: CCCCCCCOC(=O)C(C)NC(=O)CCCCCl
Molecular Weight: 305.84



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-212.40	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-677.86	kJ/mol	Joback Method
$\Delta_{fus} H°$	44.76	kJ/mol	Joback Method
$\Delta_{vap} H°$	75.32	kJ/mol	Joback Method
$logP_{oct/wat}$	3.41		Crippen Method
P_c	1519.94	kPa	Joback Method
T_{boil}	759.92	K	Joback Method
T_c	945.97	K	Joback Method
T_{fus}	448.48	K	Joback Method
V_c	0.98	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	738.55	J/mol×K	759.92	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C15H28ClNO3/c1-3-4-5-6-9-12-20-15(19)13(2)17-14(18)10-7-8-11-16/h13H,3-12H2,1-2H3,(H,17,18)

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).

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