Sarcosylsarcosine, n-propoxycarbonyl-, propyl ester

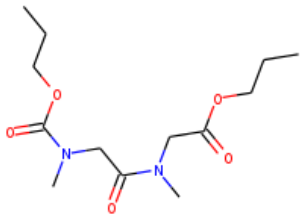
InChI: InChI=1S/C13H24N2O5/c1-5-7-19-12(17)10-14(3)11(16)9-15(4)13(18)20-8-6-2/h5-10H2,1-4H3

InChI Key: UUPQSYOFXNLOLK-UHFFFAOYSA-N

Formula: C13H24N2O5

SMILES: CCCOC(=O)CN(C)C(=O)CN(C)C(=O)OCCC

Molecular Weight: 288.34



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-316.62	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-778.77	kJ/mol	Joback Method
$\Delta_{fus} H°$	42.64	kJ/mol	Joback Method
$\Delta_{vap} H°$	73.68	kJ/mol	Joback Method
$logP_{oct/wat}$	0.88		Crippen Method
P_c	1865.94	kPa	Joback Method
T_{boil}	728.17	K	Joback Method
T_c	910.71	K	Joback Method
T_{fus}	495.46	K	Joback Method
V_c	0.85	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	669.30	J/mol×K	728.17	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C13H24N2O5/c1-5-7-19-12(17)10-14(3)11(16)9-15(4)13(18)20-8-6-2/h5-10H2,1-4H3

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).