

Sarcosylsarcosine, n-propoxycarbonyl-, undecyl ester

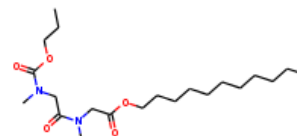
InChI: InChI=1S/C21H40N2O5/c1-5-7-8-9-10-11-12-13-14-16-27-20(25)1
8-22(3)19(24)17-23(4)21(26)28-15-6-2/h5-18H2,1-4H3

InChI Key: MTOOOSVVGZHZMD-UHFFFAOYSA-N

Formula: C₂₁H₄₀N₂O₅

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

Molecular Weight: 400.55



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-249.26	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-943.89	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	63.36	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	91.48	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	3.997		Crippen Method
P_c	1052.09	kPa	Joback Method
T_{boil}	911.21	K	Joback Method
T_c	1116.12	K	Joback Method
T_{fus}	585.62	K	Joback Method
V_c	1.302	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	1139.87	J/mol×K	911.21	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C21H40N2O5/c1-5-7-8-9-10-11-12-13-14-16-27-20\(25\)18-22\(3\)19\(24\)17-23\(4\)21\(26\)28-15-6-2/h5-18H2,1-4H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C21H40N2O5/c1-5-7-8-9-10-11-12-13-14-16-27-20(25)18-22(3)19(24)17-23(4)21(26)28-15-6-2/h5-18H2,1-4H3)

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).

$\log P_{oct/wat}$: 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 (m³/kg-mol).

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