

Sarcosylsarcosine, n-propoxycarbonyl-, octyl ester

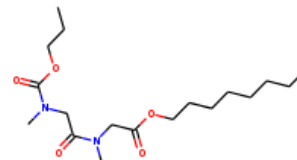
InChI: InChI=1S/C18H34N2O5/c1-5-7-8-9-10-11-13-24-17(22)15-19(3)16(21)14-20(4)18(23)25-12-6-2/h5-15H2,1-4H3

InChI Key: YMIWANUKUFZJNH-UHFFFAOYSA-N

Formula: C18H34N2O5

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

Molecular Weight: 358.47



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-274.52	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-881.97	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	55.59	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	84.81	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	2.827		Crippen Method
P_c	1280.08	kPa	Joback Method
T_{boil}	842.57	K	Joback Method
T_c	1033.26	K	Joback Method
T_{fus}	551.81	K	Joback Method
V_c	1.133	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	957.48	J/mol×K	842.57	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C18H34N2O5/c1-5-7-8-9-10-11-13-24-17\(22\)15-19\(3\)16\(21\)14-20\(4\)18\(23\)25-12-6-2/h5-15H2,1-4H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C18H34N2O5/c1-5-7-8-9-10-11-13-24-17(22)15-19(3)16(21)14-20(4)18(23)25-12-6-2/h5-15H2,1-4H3)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$C_{p, \text{gas}}$: Ideal gas heat capacity (J/mol×K).

$\Delta_f G^\circ$: Standard Gibbs free energy of formation (kJ/mol).

$\Delta_f H^\circ_{\text{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{\text{fus}} H^\circ$: Enthalpy of fusion at standard conditions (kJ/mol).

$\Delta_{\text{vap}} H^\circ$: Enthalpy of vaporization at standard conditions (kJ/mol).

$\log P_{\text{oct/wat}}$: 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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