

Sarcosine, n-valeryl-, dodecyl ester

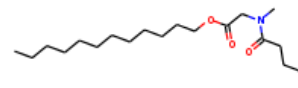
InChI: InChI=1S/C20H39NO3/c1-4-6-8-9-10-11-12-13-14-15-17-24-20(23)18-21(3)19(22)16-7-5-2/h4-18H2,1-3H3

InChI Key: AATJXMIVDDBCNG-UHFFFAOYSA-N

Formula: C20H39NO3

SMILES: CCCCCCCCCCCCCOC(=O)CN(C)C(=O)CCCC

Molecular Weight: 341.53



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-134.54	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-745.98	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	54.96	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	78.06	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	5.099		Crippen Method
P_c	1088.50	kPa	Joback Method
T_{boil}	799.60	K	Joback Method
T_c	981.59	K	Joback Method
T_{fus}	469.72	K	Joback Method
V_c	1.204	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	980.61	J/mol×K	799.6	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C20H39NO3/c1-4-6-8-9-10-11-12-13-14-15-17-24-20\(23\)18-21\(3\)19\(22\)16-7-5-2/h4-18H2,1-3H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C20H39NO3/c1-4-6-8-9-10-11-12-13-14-15-17-24-20(23)18-21(3)19(22)16-7-5-2/h4-18H2,1-3H3)

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

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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