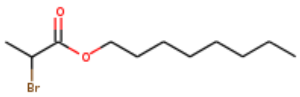
2- Bromopropionic acid, octyl ester

Other names: Octyl 2-bromopropanoate.
InChI: InChI=1S/C11H21BrO2/c1-3-4-5-6-7-8-9-14-11(13)10(2)12/h10H,3-9H2,1-2H3
InChI Key: BOCFEZOZUMAGFA-UHFFFAOYSA-N
Formula: C11H21BrO2
SMILES: CCCCCCCCOC(=O)C(C)Br
Molecular Weight: 265.19
CAS: 24625-82-9



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-180.30	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-494.12	kJ/mol	Joback Method
$\Delta_{fus} H°$	28.79	kJ/mol	Joback Method
$\Delta_{vap} H°$	55.28	kJ/mol	Joback Method
$logP_{oct/wat}$	3.674		Crippen Method
P_c	2161.32	kPa	Joback Method
T_{boil}	593.09	K	Joback Method
T_c	779.97	K	Joback Method
T_{fus}	330.69	K	Joback Method
V_c	0.732	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	462.31	J/mol×K	593.09	Joback Method
η	0.0001824	Pa×s	593.09	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C11H21BrO2/c1-3-4-5-6-7-8-9-14-11(13)10(2)12/h10H,3-9H2,1-2H3
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
η: Dynamic viscosity (Pa×s).
$\Delta_f\mathbf{G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f\mathbf{H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus}\mathbf{H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap}\mathbf{H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\boldsymbol{log}\mathbf{P_{oct/wat}}$: 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).