

Glutaric acid, monoamide, N-(2-bromophenyl)-, butyl ester

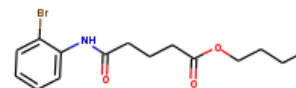
InChI: InChI=1S/C15H20BrNO3/c1-2-3-11-20-15(19)10-6-9-14(18)17-13-8-5-4-7-12(13)16/h4-5,7-8H,2-3,6,9-11H2,1H3,(H,17,18)

InChI Key: ZLVCPRSSZOYJII-UHFFFAOYSA-N

Formula: C15H20BrNO3

SMILES: CCCOC(=O)CCCC(=O)Nc1ccccc1Br

Molecular Weight: 342.23



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-80.93	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-405.45	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	43.03	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	80.70	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	3.90		Crippen Method
P_c	2161.32	kPa	Joback Method
T_{boil}	820.75	K	Joback Method
T_c	1036.51	K	Joback Method
T_{fus}	532.30	K	Joback Method
V_c	0.89	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	658.84	J/mol×K	820.75	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C15H20BrNO3/c1-2-3-11-20-15\(19\)10-6-9-14\(18\)17-13-8-5-4-7-12\(13\)16/h4-5,7-8H,2-3,6,9-11H2,1H3,\(H,17,18\)](http://webbook.nist.gov/cgi/inchi/InChI=1S/C15H20BrNO3/c1-2-3-11-20-15(19)10-6-9-14(18)17-13-8-5-4-7-12(13)16/h4-5,7-8H,2-3,6,9-11H2,1H3,(H,17,18))

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).

$logP_{oct/wat}$: 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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