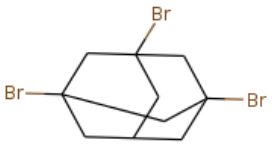
1,3,5-Tribromoadamantane

InChI:
InChI=1S/C10H13Br3/c11-8-1-7-2-9(12,4-8)6-10(13,3-7)5-8/h7H,1-6H2
InChI Key: WZCLLQRZXWUEOP-UHFFFAOYSA-N
Formula: C10H13Br3
SMILES: BrC12CC3CC(Br)(C1)CC(Br)(C3)C2
Molecular Weight: 372.92



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	222.25	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	66.88	kJ/mol	Joback Method
$\Delta_{fus} H°$	11.99	kJ/mol	Joback Method
$\Delta_{vap} H°$	53.31	kJ/mol	Joback Method
$logP_{oct/wat}$	4.39		Crippen Method
P_c	4730.11	kPa	Joback Method
T_{boil}	647.22	K	Joback Method
T_c	939.65	K	Joback Method
T_{fus}	499.62	K	Joback Method
V_c	0.64	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	399.71	J/mol×K	647.22	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C10H13Br3/c11-8-1-7-2-9(12,4-8)6-10(13,3-7)5-8/h7H,1-6H2

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

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).
$\Delta_f G°$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f H°_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus} H°$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap} H°$: 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 (m^3/kg-mol).