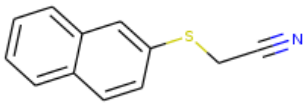
2-Naphthylthioacetonitrile

InChI: InChI=1S/C12H9NS/c13-7-8-14-12-6-5-10-3-1-2-4-11(10)9-12/h1-6,9H,8H2
InChI Key: PFMHSJMACRLMEX-UHFFFAOYSA-N
Formula: C12H9NS
SMILES: N#CCSc1ccc2ccccc2c1
Molecular Weight: 199.27
CAS: 5324-69-6



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	425.89	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	331.87	kJ/mol	Joback Method
$\Delta_{fus} H°$	23.14	kJ/mol	Joback Method
$\Delta_{vap} H°$	64.18	kJ/mol	Joback Method
$logP_{oct/wat}$	3.46		Crippen Method
P_c	3028.94	kPa	Joback Method
T_{boil}	695.46	K	Joback Method
T_c	958.30	K	Joback Method
T_{fus}	396.03	K	Joback Method
V_c	0.60	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	366.69	J/mol×K	695.46	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H9NS/c13-7-8-14-12-6-5-10-3-1-2-4-11(10)9-12/h1-6,9H,8H2

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

Legend

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

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