

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

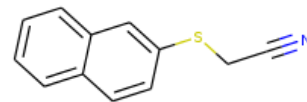
InChI Key: PFMHSJMACRLMEX-UHFFFAOYSA-N

Formula: C₁₂H₉NS

SMILES: N#CCSc1ccc2ccccc2c1

Molecular Weight: 199.27

CAS: 5324-69-6



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	425.89	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	331.87	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	23.14	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	64.18	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	3.455		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	0.602	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	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](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/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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