

Naphthol AS

Inchi:	InChI=1S/C17H13NO2/c19-16-11-13-7-5-4-6-12(13)10-15(16)17(20)18-14-8-2-1-3-9-14/
InchiKey:	JFGQHAHJWJBOPD-UHFFFAOYSA-N
Formula:	C17H13NO2
SMILES:	O=C(Nc1ccccc1)c1cc2ccccc2cc1O
Mol. weight [g/mol]:	263.30
CAS:	92-77-3

Physical Properties

Property code	Value	Unit	Source
hf	-82.60	kJ/mol	Cheméo Relay (1.0)
hfus	36.98	kJ/mol	Joback Method
ie	7.50	eV	Cheméo Relay (1.0)
log10ws	-4.43		Cheméo Relay (1.0)
logp	3.798		Crippen Method
mcvol	200.830	ml/mol	McGowan Method
tb	675.16	K	Cheméo Relay (1.0)
tf	521.65	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	-1.00290e+02
Coeff. B	1.60060e+00
Coeff. C	-1.31934e-03
Coeff. D	4.32860e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

Latest version available from:

<https://www.chemeo.com/cid/101-424-8/Naphthol-AS.pdf>

Generated by Cheméo on 2026-10-30 23:58:21.037346384 +0000 UTC m=+28413.964183637.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.