2-Naphthylacetonitrile

Other names: «beta»-Naphthyleneacetonitrile
2-Naphthaleneacetonitrile
Inchi: InChI=1S/C12H9N/c13-8-7-10-5-6-11-3-1-2-4-12(11)9-10/h1-6,9H,7H2
InchiKey: LPCWDVLDJVZIHA-UHFFFAOYSA-N
Formula: C12H9N
SMILES: N#CCc1ccc2ccccc2c1
Mol. weight [g/mol]: 167.21
CAS: 7498-57-9

Physical Properties

Property code	Value	Unit	Source
gf	392.77	kJ/mol	Joback Method
hf	290.00	kJ/mol	Joback Method
hfus	19.01	kJ/mol	Joback Method
hvap	57.36	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	2.906		Crippen Method
mcvol	138.100	ml/mol	McGowan Method
pc	2973.04	kPa	Joback Method
tb	576.20	K	NIST Webbook
tc	872.33	K	Joback Method
tf	361.63	K	Joback Method
vc	0.547	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.29	J/mol×K	626.68	Joback Method
cpg	333.25	J/mol×K	667.62	Joback Method
cpg	344.26	J/mol×K	708.56	Joback Method
cpg	354.40	J/mol×K	749.50	Joback Method
cpg	363.75	J/mol×K	790.45	Joback Method
cpg	372.41	J/mol×K	831.39	Joback Method
cpg	380.46	J/mol×K	872.33	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7498579&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume