

2-Naphthyl benzoate

Other names:	«beta»-Naphthyl benzoate Benzoic acid 2-naphthyl ester 2-Naphthalenol, benzoate «beta»-Naphthol benzoate Betabenzon 2-Benzoyloxynaphthalene 2-Naphthol, benzoate Benzoic acid, beta-naphthyl ester 2-Naphthalenol, 2-benzoate Benzonaphthol NSC 5537
Inchi:	InChI=1S/C17H12O2/c18-17(14-7-2-1-3-8-14)19-16-11-10-13-6-4-5-9-15(13)12-16/h1-12
InchiKey:	DWJIJRSTYFPKGD-UHFFFAOYSA-N
Formula:	C17H12O2
SMILES:	O=C(Oc1ccc2ccccc2c1)c1ccccc1
Mol. weight [g/mol]:	248.28
CAS:	93-44-7

Physical Properties

Property code	Value	Unit	Source
chs	-8219.90 ± 3.30	kJ/mol	NIST Webbook
gf	180.18	kJ/mol	Joback Method
hf	13.65	kJ/mol	Joback Method
hfus	27.29	kJ/mol	Joback Method
hvap	69.45	kJ/mol	Joback Method
ie	7.82	eV	NIST Webbook
log10ws	-5.36		Crippen Method
logp	4.059		Crippen Method
mcvol	190.850	ml/mol	McGowan Method
pc	2735.42	kPa	Joback Method
tb	741.97	K	Joback Method
tc	998.93	K	Joback Method
tf	381.20 ± 0.50	K	NIST Webbook
vc	0.718	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.24	J/mol×K	741.97	Joback Method
cpg	517.69	J/mol×K	784.80	Joback Method
cpg	530.85	J/mol×K	827.62	Joback Method
cpg	542.83	J/mol×K	870.45	Joback Method
cpg	553.74	J/mol×K	913.27	Joback Method
cpg	563.69	J/mol×K	956.10	Joback Method
cpg	572.80	J/mol×K	998.93	Joback Method
dvisc	0.0007434	Pa×s	499.97	Joback Method
dvisc	0.0011407	Pa×s	451.57	Joback Method
dvisc	0.0005225	Pa×s	548.37	Joback Method
dvisc	0.0003888	Pa×s	596.77	Joback Method
dvisc	0.0003025	Pa×s	645.17	Joback Method
dvisc	0.0002437	Pa×s	693.57	Joback Method
dvisc	0.0002020	Pa×s	741.97	Joback Method
hfust	26.23	kJ/mol	381.20	NIST Webbook
hfust	26.23	kJ/mol	381.20	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C93447&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions

hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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

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