1-Naphthalenol, benzoate

Other names: 1-Naphthol, benzoate
1-Naphthyl benzoate
Benzoic acid, 1-naphthyl ester
Inchi: InChI=1S/C17H12O2/c18-17(14-8-2-1-3-9-14)19-16-12-6-10-13-7-4-5-11-15(13)16/h1-12
InchiKey: KZWCTFLBFSWYHS-UHFFFAOYSA-N
Formula: C17H12O2
SMILES: O=C(Oc1cccc2ccccc12)c1ccccc1
Mol. weight [g/mol]: 248.28
CAS: 607-55-6

Physical Properties

Property code	Value	Unit	Source
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	7.81	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	329.00 ± 0.50	K	NIST Webbook
vc	0.718	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	563.69	J/mol×K	956.10	Joback Method
cpg	572.80	J/mol×K	998.93	Joback Method
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
dvisc	0.0002020	Pa×s	741.97	Joback Method
dvisc	0.0002437	Pa×s	693.57	Joback Method
dvisc	0.0011407	Pa×s	451.57	Joback Method
dvisc	0.0007434	Pa×s	499.97	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
hfust	16.98	kJ/mol	329.20	NIST Webbook
hfust	16.98	kJ/mol	329.20	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C607556&Units=SI

Legend

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