Naphthalene, 2-bromo-

Other names:	2-Bromonaphthalene
	2-Bromonapthalene
	2-Naphthyl bromide
	«beta»-Bromonaphthalene
	«beta»-Naphthyl bromide
	Â«betaÂ»-Bromonaphthalene
	Â«betaÂ»-Naphthyl bromide
Inchi:	InChI=1S/C10H7Br/c11-10-6-5-8-3-1-2-4-9(8)7-10/h1-7H
InchiKey:	APSMUYYLXZULMS-UHFFFAOYSA-N
Formula:	C10H7Br
SMILES:	Brc1ccc2ccccc2c1
Mol. weight [g/mol]:	207.07
CAS:	580-13-2

Physical Properties

Property code	Value	Unit	Source
chs	-5029.90 ± 1.70	kJ/mol	NIST Webbook
gf	257.07	kJ/mol	Joback Method
hf	175.60 ± 2.30	kJ/mol	NIST Webbook
hfs	94.40 ± 2.10	kJ/mol	NIST Webbook
hfus	17.61	kJ/mol	Joback Method
hsub	81.20 ± 1.00	kJ/mol	NIST Webbook
hsub	64.00 ± 5.00	kJ/mol	NIST Webbook
hsub	81.20 ± 1.00	kJ/mol	NIST Webbook
hvap	66.10 ± 0.40	kJ/mol	NIST Webbook
ie	8.18 ± 0.03	eV	NIST Webbook
log10ws	-4.40		Estimated Solubility Method
log10ws	-4.40		Aqueous Solubility Prediction Method
logp	3.602		Crippen Method
mcvol	126.040	ml/mol	McGowan Method
pc	4173.09	kPa	Joback Method
tb	554.70	K	NIST Webbook
tb	554.15 ± 0.70	K	NIST Webbook
tc	800.62	K	Joback Method
tf	332.00 ± 1.00	K	NIST Webbook

vc	0.471	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.39	J/mol×K	672.81	Joback Method
cpg	302.26	J/mol×K	800.62	Joback Method
cpg	294.68	J/mol×K	758.02	Joback Method
cpg	286.42	J/mol×K	715.42	Joback Method
cpg	244.65	J/mol×K	545.00	Joback Method
cpg	256.61	J/mol×K	587.60	Joback Method
cpg	267.49	J/mol×K	630.21	Joback Method
dvisc	0.0006718	Pa×s	439.45	Joback Method
dvisc	0.0003922	Pa×s	545.00	Joback Method
dvisc	0.0005467	Pa×s	474.63	Joback Method
dvisc	0.0004578	Pa×s	509.82	Joback Method
dvisc	0.0016175	Pa×s	333.90	Joback Method
dvisc	0.0011413	Pa×s	369.08	Joback Method
dvisc	0.0008557	Pa×s	404.27	Joback Method
hfust	14.40	kJ/mol	329.00	NIST Webbook
hfust	14.40	kJ/mol	329.00	NIST Webbook
hfust	5.77	kJ/mol	319.00	NIST Webbook
hvapt	40.40	kJ/mol	340.50	NIST Webbook
hvapt	42.50	kJ/mol	354.00	NIST Webbook
sfust	43.76	J/mol×K	329.00	NIST Webbook
sfust	18.09	J/mol×K	319.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C580132&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume