

2-(BROMOMETHYL)NAPHTHALENE

Other names:	«beta»-(Bromomethyl)naphthalene 2-(Bromomethyl)naphthalene 2-Menaphthyl bromide «beta»-Naphthylmethyl bromide 2-Naphthylmethyl bromide
Inchi:	InChI=1S/C11H9Br/c12-8-9-5-6-10-3-1-2-4-11(10)7-9/h1-7H,8H2
InchiKey:	RUHJZSZTSCSTCC-UHFFFAOYSA-N
Formula:	C11H9Br
SMILES:	BrCc1ccc2ccccc2c1
Mol. weight [g/mol]:	221.10

Physical Properties

Property code	Value	Unit	Source
af	0.4931		Cheméo Relay (1.0)
gf	265.49	kJ/mol	Joback Method
hf	145.98	kJ/mol	Cheméo Relay (1.0)
hfus	20.20	kJ/mol	Joback Method
hvap	73.39	kJ/mol	Cheméo Relay (1.0)
ie	8.21	eV	Cheméo Relay (1.0)
log10ws	-4.74		Cheméo Relay (1.0)
logp	3.735		Crippen Method
mcvol	140.130	ml/mol	McGowan Method
pc	3699.95	kPa	Joback Method
tb	578.84	K	Cheméo Relay (1.0)
tc	823.94	K	Cheméo Relay (1.0)
tf	366.68	K	Cheméo Relay (1.0)
vc	0.510	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.89	J/mol×K	567.88	Joback Method
cpg	352.09	J/mol×K	817.91	Joback Method
cpg	343.62	J/mol×K	776.24	Joback Method

cpg	334.46	J/mol×K	734.57	Joback Method
cpg	324.51	J/mol×K	692.89	Joback Method
cpg	313.67	J/mol×K	651.22	Joback Method
cpg	301.83	J/mol×K	609.55	Joback Method
dvisc	0.0006512	Pa×s	456.53	Joback Method
dvisc	0.0003701	Pa×s	567.88	Joback Method
dvisc	0.0004352	Pa×s	530.76	Joback Method
dvisc	0.0005243	Pa×s	493.64	Joback Method
dvisc	0.0016500	Pa×s	345.17	Joback Method
dvisc	0.0008404	Pa×s	419.41	Joback Method
dvisc	0.0011396	Pa×s	382.29	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	486.20	K	13.30	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C939264&Units=SI>

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):

Legend

af:	Acentric Factor
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

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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