NAPHTHALENE, 1,1'-METHYLENEBIS-

Inchi: InChI=1S/C21H16/c1-3-13-20-16(7-1)9-5-11-18(20)15-19-12-6-10-17-8-2-4-14-21(17)19/
InchiKey: ZMESHQOXZMOOQQ-UHFFFAOYSA-N
Formula: C21H16
SMILES: c1ccc2c(Cc3cccc4ccccc34)cccc2c1
Mol. weight [g/mol]: 268.36

Physical Properties

Property code	Value	Unit	Source
af	0.5787		Cheméo Relay (1.0)
gf	544.80	kJ/mol	Joback Method
hf	316.00	kJ/mol	Cheméo Relay (1.0)
hfus	31.49	kJ/mol	Joback Method
hvap	116.57	kJ/mol	Cheméo Relay (1.0)
ie	7.82	eV	Cheméo Relay (1.0)
log10ws	-7.48		Cheméo Relay (1.0)
logp	5.584		Crippen Method
mcvol	220.310	ml/mol	McGowan Method
pc	2241.88	kPa	Joback Method
tb	724.48	K	Cheméo Relay (1.0)
tc	1007.17	K	Cheméo Relay (1.0)
tf	408.30	K	Cheméo Relay (1.0)
vc	0.828	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	607.05	J/mol×K	781.16	Joback Method
cpg	623.40	J/mol×K	825.11	Joback Method
cpg	638.49	J/mol×K	869.05	Joback Method
cpg	652.54	J/mol×K	913.00	Joback Method
cpg	665.73	J/mol×K	956.95	Joback Method
cpg	678.29	J/mol×K	1000.89	Joback Method
cpg	690.41	J/mol×K	1044.84	Joback Method
dvisc	0.0013110	Pa×s	469.71	Joback Method

dvisc	0.0009229	Pa×s	521.62	Joback Method
dvisc	0.0006923	Pa×s	573.53	Joback Method
dvisc	0.0005447	Pa×s	625.44	Joback Method
dvisc	0.0004446	Pa×s	677.34	Joback Method
dvisc	0.0003735	Pa×s	729.25	Joback Method
dvisc	0.0003212	Pa×s	781.16	Joback Method

Sources

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C607501&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume