1,4,5,8-Dimethanonaphthalene, 1,4,4a,5,8,8a-hexahydro-, (1«alpha»,4«alpha»,4a«beta»,5«alpha»,8«alpha»,8

Inchi: InChI=1S/C12H14/c1-2-8-5-7(1)11-9-3-4-10(6-9)12(8)11/h1-4,7-12H,5-6H2/t7-,8+,9+,10

InchiKey: ZSJSHFJUHHVKQB-KUDAMMAASA-N

Formula: C12H14

SMILES: C1=CC2CC1C1C3C=CC(C3)C21

Mol. weight [g/mol]: 158.24

CAS: 83602-18-0

Physical Properties

Property code	Value	Unit	Source
gf	337.66	kJ/mol	Joback Method
hf	75.07	kJ/mol	Joback Method
hfus	23.96	kJ/mol	Joback Method
hvap	41.92	kJ/mol	Joback Method
ie	8.08	eV	NIST Webbook
ie	8.20	eV	NIST Webbook
ie	8.48 ± 0.03	eV	NIST Webbook
log10ws	-2.68		Crippen Method
logp	2.631		Crippen Method
mcvol	127.900	ml/mol	McGowan Method
pc	2940.89	kPa	Joback Method
tb	489.90	K	Joback Method
tc	710.29	K	Joback Method
tf	289.80	K	Joback Method
vc	0.505	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.54	J/mol×K	489.90	Joback Method
cpg	341.07	J/mol×K	526.63	Joback Method
cpg	359.95	J/mol×K	563.36	Joback Method
cpg	377.31	J/mol×K	600.10	Joback Method
cpg	393.29	J/mol×K	636.83	Joback Method
cpg	408.06	J/mol×K	673.56	Joback Method

cpg	421.73	J/mol×K	710.29	Joback Method
dvisc	0.0005230	Pa×s	289.80	Joback Method
dvisc	0.0008339	Pa×s	323.15	Joback Method
dvisc	0.0012184	Pa×s	356.50	Joback Method
dvisc	0.0016684	Pa×s	389.85	Joback Method
dvisc	0.0021742	Pa×s	423.20	Joback Method
dvisc	0.0027258	Pa×s	456.55	Joback Method
dvisc	0.0033138	Pa×s	489.90	Joback Method

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=C83602180&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
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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