1,4:5,8-dimethano-naphthalene,1,2,4,4a,8,8,8a-oct

Other names: Tetracyclo[6.2.1.1(3,6).0(2,7)]dodec-9-ene
Inchi: InChI=1S/C12H16/c1-2-8-5-7(1)11-9-3-4-10(6-9)12(8)11/h1-2,7-12H,3-6H2
InchiKey: XBFJAVXCNXDMBH-UHFFFAOYSA-N
Formula: C12H16
SMILES: C1=CC2CC1C1C3CCC(C3)C21
Mol. weight [g/mol]: 160.26
CAS: 21635-90-5

Physical Properties

Property code	Value	Unit	Source
gf	307.70	kJ/mol	Joback Method
hf	17.29	kJ/mol	Joback Method
hfus	22.74	kJ/mol	Joback Method
hvap	41.63	kJ/mol	Joback Method
ie	8.60	eV	NIST Webbook
ie	8.85 ± 0.03	eV	NIST Webbook
log10ws	-2.83		Crippen Method
logp	2.855		Crippen Method
mcvol	132.200	ml/mol	McGowan Method
pc	2829.33	kPa	Joback Method
tb	490.74	K	Joback Method
tc	708.89	K	Joback Method
tf	289.04	K	Joback Method
vc	0.519	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	337.17	J/mol×K	490.74	Joback Method
cpg	430.51	J/mol×K	672.53	Joback Method
cpg	414.64	J/mol×K	636.17	Joback Method
cpg	397.50	J/mol×K	599.81	Joback Method
cpg	378.97	J/mol×K	563.46	Joback Method
cpg	358.91	J/mol×K	527.10	Joback Method

cpg	445.26	J/mol×K	708.89	Joback Method
dvisc	0.0033819	Pa×s	490.74	Joback Method
dvisc	0.0028194	Pa×s	457.12	Joback Method
dvisc	0.0022834	Pa×s	423.51	Joback Method
dvisc	0.0017834	Pa×s	389.89	Joback Method
dvisc	0.0013293	Pa×s	356.27	Joback Method
dvisc	0.0009320	Pa×s	322.66	Joback Method
dvisc	0.0006017	Pa×s	289.04	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=C21635905&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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