1,4:5,8-Dimethano-4a,8a-(methanoxymethano)nap
octahydro-(1α,4α,4aβ,5β,8&

Other names: 1,4:5,8-Dimethanonaphthalene, 1,2,3,4,4a,5,8,8a-octahydro-(1«alpha»,4«alpha»,4a«beta»,5«beta»,8«alpha»,8a«beta»)-, 1,4:5,8-Dimethano-4a,8a-(methanoxymethano)naphthalene-9,11-dione, octahydro-(1«alpha»,4«alpha»,4a«beta»,5«beta»,8«alpha»,8a«beta»)-

Inchi: InChI=1S/C12H16/c1-2-8-5-7(1)11-9-3-4-10(6-9)12(8)11/h7-10H,1-6H2

InchiKey: WNOQFKCATWEQFU-UHFFFAOYSA-N

Formula: C12H16

SMILES: C1CC2CC1C1=C2C2CCC1C2

Mol. weight [g/mol]: 160.26

CAS: 73679-39-7

Physical Properties

Property code	Value	Unit	Source
gf	303.86	kJ/mol	Joback Method
hf	35.03	kJ/mol	Joback Method
hfus	19.82	kJ/mol	Joback Method
hvap	43.57	kJ/mol	Joback Method
ie	7.90	eV	NIST Webbook
ie	7.90 ± 0.02	eV	NIST Webbook
log10ws	-3.31		Crippen Method
logp	3.143		Crippen Method
mcvol	132.200	ml/mol	McGowan Method
pc	2940.89	kPa	Joback Method
tb	510.04	K	Joback Method
tc	731.02	K	Joback Method
tf	322.56	K	Joback Method
vc	0.521	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.92	J/mol×K	510.04	Joback Method
cpg	358.69	J/mol×K	546.87	Joback Method
cpg	376.91	J/mol×K	583.70	Joback Method
cpg	393.73	J/mol×K	620.53	Joback Method
cpg	409.30	J/mol×K	657.36	Joback Method

cpg	423.75	J/mol×K	694.19	Joback Method
cpg	437.23	J/mol×K	731.02	Joback Method
dvisc	0.0013184	Pa×s	322.56	Joback Method
dvisc	0.0016508	Pa×s	353.81	Joback Method
dvisc	0.0019930	Pa×s	385.05	Joback Method
dvisc	0.0023390	Pa×s	416.30	Joback Method
dvisc	0.0026845	Pa×s	447.55	Joback Method
dvisc	0.0030260	Pa×s	478.79	Joback Method
dvisc	0.0033613	Pa×s	510.04	Joback Method

Sources

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=C73679397&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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