Naphthalene,1,2,3,4,4a,5,6,8a-octahydro-8a-metho

Inchi: InChI=1S/C12H20O/c1-11-7-3-5-9-12(11,13-2)10-6-4-8-11/h5,9H,3-4,6-8,10H2,1-2H3/t1
InchiKey: RCZSDAHEJJIWKF-NWDGAFQWSA-N
Formula: C12H20O
SMILES: COC12C=CCCC1(C)CCCC2
Mol. weight [g/mol]: 180.29
CAS: 68211-38-1

Physical Properties

Property code	Value	Unit	Source
gf	37.24	kJ/mol	Joback Method
hf	-214.01	kJ/mol	Joback Method
hfus	4.52	kJ/mol	Joback Method
hvap	43.22	kJ/mol	Joback Method
ie	9.35 ± 0.02	eV	NIST Webbook
ie	9.00 ± 0.05	eV	NIST Webbook
log10ws	-3.45		Crippen Method
logp	3.302		Crippen Method
mcvol	159.790	ml/mol	McGowan Method
pc	2767.17	kPa	Joback Method
tb	526.58	K	Joback Method
tc	760.50	K	Joback Method
tf	317.59	K	Joback Method
vc	0.590	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.24	J/mol×K	526.58	Joback Method
cpg	415.88	J/mol×K	565.57	Joback Method
cpg	435.87	J/mol×K	604.55	Joback Method
cpg	454.47	J/mol×K	643.54	Joback Method
cpg	471.97	J/mol×K	682.53	Joback Method
cpg	488.62	J/mol×K	721.52	Joback Method
cpg	504.70	J/mol×K	760.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C68211381&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
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