Naphthalene,decahydro-4a-methoxy-8a-methyl-tra

Inchi: InChI=1S/C12H22O/c1-11-7-3-5-9-12(11,13-2)10-6-4-8-11/h3-10H2,1-2H3/t11-,12+
InchiKey: NTKZWUWLFVYFJS-TXEJJXNPSA-N
Formula: C12H22O
SMILES: COC12CCCCC1(C)CCCC2
Mol. weight [g/mol]: 182.30
CAS: 17987-53-0

Physical Properties

Property code	Value	Unit	Source
gf	7.28	kJ/mol	Joback Method
hf	-271.79	kJ/mol	Joback Method
hfus	3.30	kJ/mol	Joback Method
hvap	42.93	kJ/mol	Joback Method
ie	9.10 ± 0.05	eV	NIST Webbook
log10ws	-3.59		Crippen Method
logp	3.526		Crippen Method
mcvol	164.090	ml/mol	McGowan Method
pc	2665.27	kPa	Joback Method
tb	527.42	K	Joback Method
tc	758.95	K	Joback Method
tf	316.83	K	Joback Method
vc	0.604	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	412.33	J/mol×K	527.42	Joback Method
cpg	435.20	J/mol×K	566.01	Joback Method
cpg	456.39	J/mol×K	604.60	Joback Method
cpg	476.17	J/mol×K	643.18	Joback Method
cpg	494.79	J/mol×K	681.77	Joback Method
cpg	512.53	J/mol×K	720.36	Joback Method
cpg	529.62	J/mol×K	758.95	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=C17987530&Units=SI

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