1-Isopropenylnaphthalene

Other names: Naphthalene, 1-methylethenyl
Inchi: InChI=1S/C13H12/c1-10(2)12-9-5-7-11-6-3-4-8-13(11)12/h3-9H,1H2,2H3
InchiKey: LCJNYCWJKAWZKZ-UHFFFAOYSA-N
Formula: C13H12
SMILES: C=C(C)c1cccc2ccccc12
Mol. weight [g/mol]: 168.23
CAS: 1855-47-6

Physical Properties

Property code	Value	Unit	Source
gf	347.30	kJ/mol	Joback Method
hf	220.12	kJ/mol	Joback Method
hfus	17.51	kJ/mol	Joback Method
hvap	48.52	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	3.873		Crippen Method
mcvol	146.510	ml/mol	McGowan Method
pc	2896.73	kPa	Joback Method
rinpol	1500.00		NIST Webbook
rinpol	257.00		NIST Webbook
tb	544.04	K	Joback Method
tc	779.75	K	Joback Method
tf	292.19	K	Joback Method
vc	0.559	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.83	J/mol×K	544.04	Joback Method
cpg	338.43	J/mol×K	583.32	Joback Method
cpg	352.85	J/mol×K	622.61	Joback Method
cpg	366.18	J/mol×K	661.89	Joback Method
cpg	378.51	J/mol×K	701.18	Joback Method
cpg	389.93	J/mol×K	740.46	Joback Method

cpg	400.53	J/mol×K	779.75	Joback Method

Sources

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=C1855476&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume