

Benzene, 1-heptenyl-, (E)

Inchi:	InChI=1S/C13H18/c1-2-3-4-5-7-10-13-11-8-6-9-12-13/h6-12H,2-5H2,1H3/b10-7+
InchiKey:	PNLSTDKQAPNMDU-JXMROGBWSA-N
Formula:	C13H18
SMILES:	CCCCC=Cc1ccccc1
Mol. weight [g/mol]:	174.28
CAS:	10201-58-8

Physical Properties

Property code	Value	Unit	Source
gf	251.21	kJ/mol	Joback Method
hf	42.10	kJ/mol	Joback Method
hfus	23.67	kJ/mol	Joback Method
hvap	46.77	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	4.280		Crippen Method
mcvol	165.970	ml/mol	McGowan Method
pc	2304.74	kPa	Joback Method
rinpol	1406.00		NIST Webbook
tb	527.68	K	Joback Method
tc	733.25	K	Joback Method
tf	257.61	K	Joback Method
vc	0.635	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.09	J/molxK	527.68	Joback Method
cpg	392.31	J/molxK	561.94	Joback Method
cpg	408.52	J/molxK	596.20	Joback Method
cpg	423.76	J/molxK	630.46	Joback Method
cpg	438.09	J/molxK	664.72	Joback Method
cpg	451.55	J/molxK	698.98	Joback Method
cpg	464.21	J/molxK	733.25	Joback Method
dvisc	0.0035385	Paxs	257.61	Joback Method

dvisc	0.0014508	Paxs	302.62	Joback Method
dvisc	0.0007493	Paxs	347.63	Joback Method
dvisc	0.0004503	Paxs	392.64	Joback Method
dvisc	0.0003005	Paxs	437.66	Joback Method
dvisc	0.0002163	Paxs	482.67	Joback Method
dvisc	0.0001646	Paxs	527.68	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=C10201588&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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

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