

Benzene, 1-ethyl-2-heptyl

Inchi:	InChI=1S/C15H24/c1-3-5-6-7-8-12-15-13-10-9-11-14(15)4-2/h9-11,13H,3-8,12H2,1-2H3
InchiKey:	CIAWMJWJMGRNQQ-UHFFFAOYSA-N
Formula:	C15H24
SMILES:	CCCCCCCc1cccc1CC
Mol. weight [g/mol]:	204.35

Physical Properties

Property code	Value	Unit	Source
gf	178.20	kJ/mol	Joback Method
hf	-127.87	kJ/mol	Joback Method
hfus	28.26	kJ/mol	Joback Method
hvap	51.92	kJ/mol	Joback Method
log10ws	-5.17		Crippen Method
logp	4.762		Crippen Method
mvol	198.450	ml/mol	McGowan Method
pc	1823.17	kPa	Joback Method
rinpol	1496.00		NIST Webbook
rinpol	1496.00		NIST Webbook
tb	574.26	K	Joback Method
tc	766.81	K	Joback Method
tf	297.75	K	Joback Method
vc	0.767	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	493.06	J/molxK	574.26	Joback Method
cpg	511.45	J/molxK	606.35	Joback Method
cpg	528.91	J/molxK	638.44	Joback Method
cpg	545.48	J/molxK	670.54	Joback Method
cpg	561.18	J/molxK	702.63	Joback Method
cpg	576.06	J/molxK	734.72	Joback Method
cpg	590.13	J/molxK	766.81	Joback Method
dvisc	0.0025521	Paxs	297.75	Joback Method

dvisc	0.0011846	Paxs	343.83	Joback Method
dvisc	0.0006592	Paxs	389.92	Joback Method
dvisc	0.0004153	Paxs	436.00	Joback Method
dvisc	0.0002857	Paxs	482.09	Joback Method
dvisc	0.0002099	Paxs	528.17	Joback Method
dvisc	0.0001620	Paxs	574.26	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=R13656&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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

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