

(3-Heptyl)benzene

Inchi:	InChI=1S/C13H20/c1-3-5-9-12(4-2)13-10-7-6-8-11-13/h6-8,10-12H,3-5,9H2,1-2H3
InchiKey:	QXZANYPVYZTYBN-UHFFFAOYSA-N
Formula:	C13H20
SMILES:	CCCCC(CC)c1ccccc1
Mol. weight [g/mol]:	176.30
CAS:	2132-85-6

Physical Properties

Property code	Value	Unit	Source
gf	168.55	kJ/mol	Joback Method
hf	-80.40	kJ/mol	Joback Method
hfus	19.94	kJ/mol	Joback Method
hvap	46.42	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	4.370		Crippen Method
mvol	170.270	ml/mol	McGowan Method
pc	2210.37	kPa	Joback Method
tb	523.08	K	Joback Method
tc	723.93	K	Joback Method
tf	247.69	K	Joback Method
vc	0.649	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.03	J/mol×K	523.08	Joback Method
cpg	473.71	J/mol×K	690.45	Joback Method
cpg	459.38	J/mol×K	656.98	Joback Method
cpg	444.18	J/mol×K	623.50	Joback Method
cpg	428.08	J/mol×K	590.03	Joback Method
cpg	411.05	J/mol×K	556.55	Joback Method
cpg	487.22	J/mol×K	723.93	Joback Method
dvisc	0.0001832	Paxs	523.08	Joback Method
dvisc	0.0002461	Paxs	477.18	Joback Method

dvisc	0.0003521	Paxs	431.28	Joback Method
dvisc	0.0005486	Paxs	385.38	Joback Method
dvisc	0.0009636	Paxs	339.49	Joback Method
dvisc	0.0020186	Paxs	293.59	Joback Method
dvisc	0.0055617	Paxs	247.69	Joback Method

Sources

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=C2132856&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	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:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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