

Benzene, 1-propylhexyl

Inchi:	InChI=1S/C15H24/c1-3-5-7-11-14(10-4-2)15-12-8-6-9-13-15/h6,8-9,12-14H,3-5,7,10-11H
InchiKey:	RTZXJZXSKXQSPQ-UHFFFAOYSA-N
Formula:	C15H24
SMILES:	CCCCC(CCC)c1ccccc1
Mol. weight [g/mol]:	204.35
CAS:	65185-83-3

Physical Properties

Property code	Value	Unit	Source
gf	185.39	kJ/mol	Joback Method
hf	-121.68	kJ/mol	Joback Method
hfus	25.12	kJ/mol	Joback Method
hvap	50.87	kJ/mol	Joback Method
log10ws	-5.17		Crippen Method
logp	5.151		Crippen Method
mvol	198.450	ml/mol	McGowan Method
pc	1859.51	kPa	Joback Method
rinpol	1443.00		NIST Webbook
tb	568.84	K	Joback Method
tc	764.22	K	Joback Method
tf	270.23	K	Joback Method
vc	0.761	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.85	J/molxK	568.84	Joback Method
cpg	511.93	J/molxK	601.40	Joback Method
cpg	530.00	J/molxK	633.97	Joback Method
cpg	547.09	J/molxK	666.53	Joback Method
cpg	563.24	J/molxK	699.10	Joback Method
cpg	578.50	J/molxK	731.66	Joback Method
cpg	592.90	J/molxK	764.22	Joback Method
dvisc	0.0050617	Paxs	270.23	Joback Method

dvisc	0.0018025	Paxs	320.00	Joback Method
dvisc	0.0008475	Paxs	369.77	Joback Method
dvisc	0.0004766	Paxs	419.54	Joback Method
dvisc	0.0003028	Paxs	469.30	Joback Method
dvisc	0.0002099	Paxs	519.07	Joback Method
dvisc	0.0001551	Paxs	568.84	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=C65185833&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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