

Benzene, hexapropyl-

Other names:	Hexapropylbenzene
Inchi:	InChI=1S/C24H42/c1-7-13-19-20(14-8-2)22(16-10-4)24(18-12-6)23(17-11-5)21(19)15-9-3
InchiKey:	VKYYKQNLHDHRHNN-UHFFFAOYSA-N
Formula:	C24H42
SMILES:	CCCCc1c(CCC)c(CCC)c(CCC)c(CCC)c1CCC
Mol. weight [g/mol]:	330.59
CAS:	2456-68-0

Physical Properties

Property code	Value	Unit	Source
gf	215.46	kJ/mol	Joback Method
hf	-359.51	kJ/mol	Joback Method
hfus	50.01	kJ/mol	Joback Method
hvap	74.60	kJ/mol	Joback Method
log10ws	-8.80		Crippen Method
logp	7.402		Crippen Method
mcvol	325.260	ml/mol	McGowan Method
pc	937.49	kPa	Joback Method
tb	800.10	K	Joback Method
tc	988.35	K	Joback Method
tf	449.26	K	Joback Method
vc	1.272	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1008.76	J/mol×K	800.10	Joback Method
cpg	1029.54	J/mol×K	831.48	Joback Method
cpg	1049.26	J/mol×K	862.85	Joback Method
cpg	1067.95	J/mol×K	894.23	Joback Method
cpg	1085.64	J/mol×K	925.60	Joback Method
cpg	1102.36	J/mol×K	956.98	Joback Method
cpg	1118.15	J/mol×K	988.35	Joback Method
dvisc	0.0006076	Pa×s	449.26	Joback Method

dvisc	0.0003329	Pa×s	507.73	Joback Method
dvisc	0.0002065	Pa×s	566.21	Joback Method
dvisc	0.0001401	Pa×s	624.68	Joback Method
dvisc	0.0001015	Pa×s	683.15	Joback Method
dvisc	0.0000774	Pa×s	741.63	Joback Method
dvisc	0.0000615	Pa×s	800.10	Joback Method
hvapt	68.40	kJ/mol	532.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.44403e+01
Coeff. B	-5.34874e+03
Coeff. C	-1.31580e+02
Temperature range (K), min.	509.51
Temperature range (K), max.	717.49

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2456680&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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