

Benzene, 1-(1,5-dimethylhexyl)-4-methyl-

Other names:	Dihydrocurcumene 1-Methyl-4-(6-methylheptan-2-yl)benzene Heptane, 2-methyl-6-p-tolyl- «alpha»-Curcumene, dihydro- 4-(1,5-Dimethylhexyl)toluene Dihydro-ar-curcumene
Inchi:	InChI=1S/C15H24/c1-12(2)6-5-7-14(4)15-10-8-13(3)9-11-15/h8-12,14H,5-7H2,1-4H3
InchiKey:	GVCHCLNHTASCCP-UHFFFAOYSA-N
Formula:	C15H24
SMILES:	<chem>Cc1ccc(C(C)CCCC(C)C)cc1</chem>
Mol. weight [g/mol]:	204.35
CAS:	1461-02-5

Physical Properties

Property code	Value	Unit	Source
gf	173.32	kJ/mol	Joback Method
hf	-138.43	kJ/mol	Joback Method
hfus	21.21	kJ/mol	Joback Method
hvap	51.15	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	4.925		Crippen Method
mcvol	198.450	ml/mol	McGowan Method
pc	1848.33	kPa	Joback Method
rinpol	1448.00		NIST Webbook
rinpol	250.03		NIST Webbook
rinpol	247.98		NIST Webbook
rinpol	243.24		NIST Webbook
rinpol	245.40		NIST Webbook
ripol	1696.00		NIST Webbook
ripol	1696.00		NIST Webbook
tb	573.38	K	Joback Method
tc	773.72	K	Joback Method
tf	267.75	K	Joback Method
vc	0.755	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	493.68	J/molxK	573.38	Joback Method
cpg	580.06	J/molxK	740.33	Joback Method
cpg	564.68	J/molxK	706.94	Joback Method
cpg	548.39	J/molxK	673.55	Joback Method
cpg	531.15	J/molxK	640.16	Joback Method
cpg	512.93	J/molxK	606.77	Joback Method
cpg	594.57	J/molxK	773.72	Joback Method
dvisc	0.0001420	Paxs	573.38	Joback Method
dvisc	0.0001922	Paxs	522.44	Joback Method
dvisc	0.0002778	Paxs	471.50	Joback Method
dvisc	0.0004389	Paxs	420.56	Joback Method
dvisc	0.0007866	Paxs	369.63	Joback Method
dvisc	0.0016990	Paxs	318.69	Joback Method
dvisc	0.0049185	Paxs	267.75	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=C1461025&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

mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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