

4-Iodopentylbenzene

Other names:	Benzene, 1-iodo-4-pentyl- 1-(4-iodophenyl)pentane
Inchi:	InChI=1S/C11H15I/c1-2-3-4-5-10-6-8-11(12)9-7-10/h6-9H,2-5H2,1H3
InchiKey:	MTRMOYSZRPLAOL-UHFFFAOYSA-N
Formula:	C11H15I
SMILES:	CCCCCc1ccc(I)cc1
Mol. weight [g/mol]:	274.14
CAS:	85017-60-3

Physical Properties

Property code	Value	Unit	Source
gf	202.64	kJ/mol	Joback Method
hf	31.56	kJ/mol	Joback Method
hfus	22.30	kJ/mol	Joback Method
hvap	52.39	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	4.024		Crippen Method
mvol	167.910	ml/mol	McGowan Method
pc	2550.76	kPa	Joback Method
tb	575.88	K	Joback Method
tc	809.46	K	Joback Method
tf	310.73	K	Joback Method
vc	0.631	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.65	J/molxK	575.88	Joback Method
cpg	371.50	J/molxK	614.81	Joback Method
cpg	385.36	J/molxK	653.74	Joback Method
cpg	398.30	J/molxK	692.67	Joback Method
cpg	410.37	J/molxK	731.60	Joback Method
cpg	421.62	J/molxK	770.53	Joback Method
cpg	432.11	J/molxK	809.46	Joback Method

dvisc	0.0027599	Paxs	310.73	Joback Method
dvisc	0.0014057	Paxs	354.92	Joback Method
dvisc	0.0008313	Paxs	399.11	Joback Method
dvisc	0.0005459	Paxs	443.31	Joback Method
dvisc	0.0003869	Paxs	487.50	Joback Method
dvisc	0.0002903	Paxs	531.69	Joback Method
dvisc	0.0002277	Paxs	575.88	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C85017603&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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