

2,5-Dibromobiphenyl

Other names:	1,1'-Biphenyl, 2,5-dibromo
Inchi:	InChI=1S/C12H8Br2/c13-10-6-7-12(14)11(8-10)9-4-2-1-3-5-9/h1-8H
InchiKey:	MHQCPXUMZCNOSF-UHFFFAOYSA-N
Formula:	C12H8Br2
SMILES:	<chem>Brc1ccc(Br)c(-c2ccccc2)c1</chem>
Mol. weight [g/mol]:	312.00
CAS:	57422-77-2

Physical Properties

Property code	Value	Unit	Source
gf	284.36	kJ/mol	Joback Method
hf	211.77	kJ/mol	Joback Method
hfus	24.71	kJ/mol	Joback Method
hvap	61.05	kJ/mol	Joback Method
log10ws	-6.40		Crippen Method
logp	4.879		Crippen Method
mcvol	167.420	ml/mol	McGowan Method
pc	3906.25	kPa	Joback Method
tb	669.60	K	Joback Method
tc	948.64	K	Joback Method
tf	422.48	K	Joback Method
vc	0.616	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.29	J/molxK	669.60	Joback Method
cpg	359.51	J/molxK	716.11	Joback Method
cpg	370.57	J/molxK	762.61	Joback Method
cpg	380.59	J/molxK	809.12	Joback Method
cpg	389.70	J/molxK	855.63	Joback Method
cpg	398.01	J/molxK	902.14	Joback Method
cpg	405.64	J/molxK	948.64	Joback Method
dvisc	0.0010809	Paxs	422.48	Joback Method

dvisc	0.0007137	Paxs	463.67	Joback Method
dvisc	0.0005042	Paxs	504.85	Joback Method
dvisc	0.0003754	Paxs	546.04	Joback Method
dvisc	0.0002913	Paxs	587.23	Joback Method
dvisc	0.0002337	Paxs	628.41	Joback Method
dvisc	0.0001927	Paxs	669.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C57422772&Units=SI
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

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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ 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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