2,2',5,5'-Tetrabromobiphenyl

Inchi:	InChI=1S/C12H6Br4/c13-7-1-3-11(15)9(5-7)10-6-8(14)2-4-12(10)16/h1-6H
InchiKey:	XEFMFJLRXHQLEM-UHFFFAOYSA-N
Formula:	C12H6Br4
SMILES:	Brc1ccc(Br)c(-c2cc(Br)ccc2Br)c1
Mol. weight [g/mol]:	469.79
CAS:	59080-37-4

Physical Properties

Property code	Value	Unit	Source
gf	293.74	kJ/mol	Joback Method
hf	241.49	kJ/mol	Joback Method
hfus	34.50	kJ/mol	Joback Method
hvap	75.25	kJ/mol	Joback Method
log10ws	-8.06		Aqueous Solubility Prediction Method
logp	6.404		Crippen Method
mcvol	202.420	ml/mol	McGowan Method
pc	4492.23	kPa	Joback Method
tb	811.88	K	Joback Method
tc	1111.87	K	Joback Method
tf	567.12	K	Joback Method
vc	0.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.65	J/mol×K	811.88	Joback Method
cpg	404.43	J/mol×K	861.88	Joback Method
cpg	412.49	J/mol×K	911.88	Joback Method
cpg	420.02	J/mol×K	961.87	Joback Method
cpg	427.16	J/mol×K	1011.87	Joback Method
cpg	434.09	J/mol×K	1061.87	Joback Method
cpg	440.97	J/mol×K	1111.87	Joback Method
dvisc	0.0004823	Pa×s	567.12	Joback Method

dvisc	0.0003613	Pa×s	607.91	Joback Method
dvisc	0.0002807	Pa×s	648.71	Joback Method
dvisc	0.0002246	Pa×s	689.50	Joback Method
dvisc	0.0001843	Pa×s	730.29	Joback Method
dvisc	0.0001544	Pa×s	771.09	Joback Method
dvisc	0.0001317	Pa×s	811.88	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C59080374&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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