2,4,6-Tribromobiphenyl

Inchi: InChI=1S/C12H7Br3/c13-9-6-10(14)12(11(15)7-9)8-4-2-1-3-5-8/h1-7H
InchiKey: YCLZBYQDXVJFII-UHFFFAOYSA-N
Formula: C12H7Br3
SMILES: Brc1cc(Br)c(-c2ccccc2)c(Br)c1
Mol. weight [g/mol]: 390.90
CAS: 59080-33-0

Physical Properties

Property code	Value	Unit	Source
gf	289.05	kJ/mol	Joback Method
hf	226.63	kJ/mol	Joback Method
hfus	29.61	kJ/mol	Joback Method
hvap	68.15	kJ/mol	Joback Method
log10ws	-7.30		Aqueous Solubility Prediction Method
logp	5.641		Crippen Method
mcvol	184.920	ml/mol	McGowan Method
pc	4183.90	kPa	Joback Method
tb	740.74	K	Joback Method
tc	1031.10	K	Joback Method
tf	494.80	K	Joback Method
vc	0.677	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.57	J/mol×K	740.74	Joback Method
cpg	416.95	J/mol×K	982.71	Joback Method
cpg	409.64	J/mol×K	934.31	Joback Method
cpg	401.79	J/mol×K	885.92	Joback Method
cpg	393.25	J/mol×K	837.53	Joback Method
cpg	383.89	J/mol×K	789.13	Joback Method
cpg	423.87	J/mol×K	1031.10	Joback Method
dvisc	0.0001631	Pa×s	740.74	Joback Method

dvisc	0.0001942	Pa×s	699.75	Joback Method
dvisc	0.0002364	Pa×s	658.76	Joback Method
dvisc	0.0002952	Pa×s	617.77	Joback Method
dvisc	0.0003806	Pa×s	576.78	Joback Method
dvisc	0.0005101	Pa×s	535.79	Joback Method
dvisc	0.0007176	Pa×s	494.80	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C59080330&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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