2,4,4'-Tribromodiphenyl ether

Other names: PBDE Congener No. 28
Inchi: InChI=1S/C12H7Br3O/c13-8-1-4-10(5-2-8)16-12-6-3-9(14)7-11(12)15/h1-7H
InchiKey: UPNBETHEXPIWQX-UHFFFAOYSA-N
Formula: C12H7Br3O
SMILES: Brc1ccc(Oc2ccc(Br)cc2Br)cc1
Mol. weight [g/mol]: 406.89
CAS: 41318-75-6

Physical Properties

Property code	Value	Unit	Source
gf	184.05	kJ/mol	Joback Method
hf	94.41	kJ/mol	Joback Method
hfus	30.79	kJ/mol	Joback Method
hvap	70.56	kJ/mol	Joback Method
log10ws	-6.60		Crippen Method
logp	5.766		Crippen Method
mcvol	190.790	ml/mol	McGowan Method
pc	4093.38	kPa	Joback Method
tb	763.16	K	Joback Method
tc	1047.35	K	Joback Method
tf	517.03	K	Joback Method
vc	0.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	444.23	J/mol×K	1047.35	Joback Method
cpg	437.96	J/mol×K	999.99	Joback Method
cpg	431.11	J/mol×K	952.62	Joback Method
cpg	423.60	J/mol×K	905.26	Joback Method
cpg	415.31	J/mol×K	857.89	Joback Method
cpg	406.16	J/mol×K	810.53	Joback Method
cpg	396.04	J/mol×K	763.16	Joback Method
dvisc	0.0005308	Pa×s	517.03	Joback Method

dvisc	0.0001241	Pa×s	763.16	Joback Method
dvisc	0.0001476	Pa×s	722.14	Joback Method
dvisc	0.0001792	Pa×s	681.12	Joback Method
dvisc	0.0002232	Pa×s	640.10	Joback Method
dvisc	0.0002863	Pa×s	599.07	Joback Method
dvisc	0.0003811	Pa×s	558.05	Joback Method
hvapt	94.10	kJ/mol	439.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C41318756&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
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
hvapt: Enthalpy of vaporization at a given temperature
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