Propane, 1-(2,4,6-tribromophenoxy)-2,3-dibromo-

Other names: 1,3,5-tribromo(2,3-dibromopropoxy)benzene
1,3,5-tribromo-2-(2,3-dibromopropoxy)benzene
2,3-Dibromopropyl 2,4,6-tribromophenyl ether
Benzene, 1,3,5-tribromo-2-(2,3-dibromopropoxy)-
Propane, 2,3-dibromo-(2,4,6-tribromophenoxy)-

Inchi: InChI=1S/C9H7Br5O/c10-3-6(12)4-15-9-7(13)1-5(11)2-8(9)14/h1-2,6H,3-4H2

InchiKey: QXWYPAKUEHGJSG-UHFFFAOYSA-N

Formula: C9H7Br5O

SMILES: BrCC(Br)COc1c(Br)cc(Br)cc1Br

Mol. weight [g/mol]: 530.67

CAS: 35109-60-5

Physical Properties

Property code	Value	Unit	Source
gf	72.58	kJ/mol	Joback Method
hf	-32.82	kJ/mol	Joback Method
hfus	36.03	kJ/mol	Joback Method
hvap	74.09	kJ/mol	Joback Method
log10ws	-6.89		Crippen Method
logp	5.511		Crippen Method
mcvol	207.280	ml/mol	McGowan Method
pc	4691.31	kPa	Joback Method
tb	799.72	K	Joback Method
tc	1076.12	K	Joback Method
tf	561.40	K	Joback Method
tt	307.90	K	Measurement of Vapor Pressures and Melting Properties of Five Polybrominated Aromatic Flame Retardants
vc	0.753	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	390.54	J/mol×K	799.72	Joback Method
cpg	424.27	J/mol×K	1030.06	Joback Method
cpg	418.28	J/mol×K	983.99	Joback Method
cpg	412.01	J/mol×K	937.92	Joback Method
cpg	405.36	J/mol×K	891.85	Joback Method
cpg	398.24	J/mol×K	845.79	Joback Method
cpg	430.06	J/mol×K	1076.12	Joback Method
dvisc	0.0001017	Pa×s	799.72	Joback Method
dvisc	0.0001208	Pa×s	760.00	Joback Method
dvisc	0.0001461	Pa×s	720.28	Joback Method
dvisc	0.0001806	Pa×s	680.56	Joback Method
dvisc	0.0002293	Pa×s	640.84	Joback Method
dvisc	0.0003005	Pa×s	601.12	Joback Method
dvisc	0.0004091	Pa×s	561.40	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Measurement of Vapor Pressures and Melting Properties of Five Polybrominated Aromatic Flame Retardants: https://www.doi.org/10.1021/acs.jced.7b01040

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=C35109605&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
tt:	Triple Point Temperature
vc:	Critical Volume