Propane, 2,2-bis[4-(2,3-dibromopropoxy)-3,5-dibromopheny

Other names: 1,1'-(isopropylidene)bis[3,5-dibromo-4-(2,3-dibromopropoxy)benzene]
2,2-bis[3,5-dibromo-4-(2,3-dibromopropyloxy)phenyl]propane

Inchi: InChI=1S/C21H20Br8O2/c1-21(2,11-3-15(26)19(16(27)4-11)30-9-13(24)7-22)12-5-17(28

InchiKey: LXIZRZRTWSDLKK-UHFFFAOYSA-N

Formula: C21H20Br8O2

SMILES: CC(C)(c1cc(Br)c(OCC(Br)CBr)c(Br)c1)c1cc(Br)c(OCC(Br)CBr)c(Br)c1

Mol. weight [g/mol]: 943.61

CAS: 21850-44-2

Physical Properties

Property code	Value	Unit	Source
gf	195.50	kJ/mol	Joback Method
hf	-145.64	kJ/mol	Joback Method
hfus	66.09	kJ/mol	Joback Method
hvap	125.09	kJ/mol	Joback Method
log10ws	-12.60		Crippen Method
logp	10.137		Crippen Method
mcvol	410.970	ml/mol	McGowan Method
pc	2248.26	kPa	Joback Method
tb	1333.13	K	Joback Method
tc	1637.55	K	Joback Method
tf	949.67	K	Joback Method
vc	1.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1056.93	J/mol×K	1333.13	Joback Method
cpg	1073.43	J/mol×K	1383.87	Joback Method
cpg	1091.20	J/mol×K	1434.60	Joback Method
cpg	1110.55	J/mol×K	1485.34	Joback Method
cpg	1131.76	J/mol×K	1536.07	Joback Method
cpg	1155.13	J/mol×K	1586.81	Joback Method
cpg	1180.95	J/mol×K	1637.55	Joback Method

dvisc	0.0000118	Pa×s	949.67	Joback Method
dvisc	0.0000085	Pa×s	1013.58	Joback Method
dvisc	0.0000064	Pa×s	1077.49	Joback Method
dvisc	0.0000050	Pa×s	1141.40	Joback Method
dvisc	0.0000040	Pa×s	1205.31	Joback Method
dvisc	0.0000032	Pa×s	1269.22	Joback Method
dvisc	0.0000027	Pa×s	1333.13	Joback Method

Sources

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=C21850442&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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