

Benzene, 1,1',1''-(bromomethyldyne)tris-

Other names:

Methane, bromotriphenyl-
«alpha»-Bromotriphenylmethane
Bromotriphenylmethane
Triphenylmethyl bromide
Trityl bromide
2-bromo-1,1,1-triphenylethane

Inchi:

InChI=1S/C19H15Br/c20-19(16-10-4-1-5-11-16,17-12-6-2-7-13-17)18-14-8-3-9-15-18/h1

InchiKey:

NZHXEWZGTQSYJM-UHFFFAOYSA-N

Formula:

C₁₉H₁₅Br

SMILES:

BrC(c1ccccc1)(c1ccccc1)c1ccccc1

Mol. weight [g/mol]:

323.23

CAS:

596-43-0

Physical Properties

Property code	Value	Unit	Source
gf	463.49	kJ/mol	Joback Method
hf	291.68	kJ/mol	Joback Method
hfus	24.96	kJ/mol	Joback Method
hvap	69.86	kJ/mol	Joback Method
log10ws	-5.89		Crippen Method
logp	5.373		Crippen Method
mcvol	224.790	ml/mol	McGowan Method
pc	2600.43	kPa	Joback Method
tb	777.09	K	Joback Method
tc	1066.21	K	Joback Method
tf	445.37	K	Joback Method
vc	0.827	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.04	J/mol×K	777.09	Joback Method
cpg	606.61	J/mol×K	825.28	Joback Method
cpg	621.49	J/mol×K	873.46	Joback Method

cpg	634.96	J/molxK	921.65	Joback Method
cpg	647.28	J/molxK	969.84	Joback Method
cpg	658.71	J/molxK	1018.02	Joback Method
cpg	669.52	J/molxK	1066.21	Joback Method
dvisc	0.0010809	Paxs	445.37	Joback Method
dvisc	0.0005500	Paxs	500.66	Joback Method
dvisc	0.0003201	Paxs	555.94	Joback Method
dvisc	0.0002055	Paxs	611.23	Joback Method
dvisc	0.0001419	Paxs	666.52	Joback Method
dvisc	0.0001038	Paxs	721.80	Joback Method
dvisc	0.0000793	Paxs	777.09	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	503.20	K	2.00	NIST Webbook

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=C596430&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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