

Triphenylmethylbromide

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

Physical Properties

Property code	Value	Unit	Source
af	0.5150		Cheméo Relay (1.0)
gf	463.49	kJ/mol	Joback Method
hf	352.10	kJ/mol	Cheméo Relay (1.0)
hfus	24.96	kJ/mol	Joback Method
hvap	93.06	kJ/mol	Cheméo Relay (1.0)
ie	8.62	eV	Cheméo Relay (1.0)
log10ws	-6.01		Cheméo Relay (1.0)
logp	5.373		Crippen Method
mcvol	224.790	ml/mol	McGowan Method
pc	2600.43	kPa	Joback Method
tb	644.47	K	Cheméo Relay (1.0)
tc	923.96	K	Cheméo Relay (1.0)
tf	415.46	K	Cheméo Relay (1.0)
vc	0.790	m3/kmol	Cheméo Relay (1.0)

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/mol×K	921.65	Joback Method
cpg	647.28	J/mol×K	969.84	Joback Method
cpg	658.71	J/mol×K	1018.02	Joback Method
cpg	669.52	J/mol×K	1066.21	Joback Method
dvisc	0.0010809	Pa×s	445.37	Joback Method
dvisc	0.0005500	Pa×s	500.66	Joback Method
dvisc	0.0003201	Pa×s	555.94	Joback Method
dvisc	0.0002055	Pa×s	611.23	Joback Method
dvisc	0.0001419	Pa×s	666.52	Joback Method
dvisc	0.0001038	Pa×s	721.80	Joback Method
dvisc	0.0000793	Pa×s	777.09	Joback Method

Pressure Dependent Properties

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

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C596430&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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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