benzene, 1,3,5-tris(bromomethyl)-

Other names: 1,3,5-tris(bromomethyl)benzene
Inchi: InChI=1S/C9H9Br3/c10-4-7-1-8(5-11)3-9(2-7)6-12/h1-3H,4-6H2
InchiKey: GHITVUOBZBZMND-UHFFFAOYSA-N
Formula: C9H9Br3
SMILES: BrCc1cc(CBr)cc(CBr)c1
Mol. weight [g/mol]: 356.88

Physical Properties

Property code	Value	Unit	Source
gf	161.01	kJ/mol	Joback Method
hf	63.49	kJ/mol	Joback Method
hfus	28.18	kJ/mol	Joback Method
hvap	58.53	kJ/mol	Joback Method
log10ws	-5.40		Crippen Method
logp	4.371		Crippen Method
mcvol	166.410	ml/mol	McGowan Method
pc	4036.37	kPa	Joback Method
rinpol	1968.00		NIST Webbook
rinpol	1968.00		NIST Webbook
tb	640.44	K	Joback Method
tc	895.18	K	Joback Method
tf	422.05	K	Joback Method
vc	0.618	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	319.60	J/mol×K	640.44	Joback Method
cpg	329.80	J/mol×K	682.90	Joback Method
cpg	339.21	J/mol×K	725.35	Joback Method
cpg	347.89	J/mol×K	767.81	Joback Method
cpg	355.95	J/mol×K	810.27	Joback Method
cpg	363.44	J/mol×K	852.73	Joback Method
cpg	370.46	J/mol×K	895.18	Joback Method

dvisc	0.0011120	Pa×s	422.05	Joback Method
dvisc	0.0007715	Pa×s	458.45	Joback Method
dvisc	0.0005649	Pa×s	494.85	Joback Method
dvisc	0.0004316	Pa×s	531.25	Joback Method
dvisc	0.0003414	Pa×s	567.64	Joback Method
dvisc	0.0002778	Pa×s	604.04	Joback Method
dvisc	0.0002314	Pa×s	640.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U402556&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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume