

Benzene, 1,1'-(bromomethylene)bis-

Other names:	Methane, bromodiphenyl- «alpha»-Bromodiphenylmethane Benzhydryl bromide Bromodiphenylmethane Diphenylbromomethane Diphenylmethyl bromide UN 1770 NSC 39226
Inchi:	InChI=1S/C13H11Br/c14-13(11-7-3-1-4-8-11)12-9-5-2-6-10-12/h1-10,13H
InchiKey:	OQROAIRCEOBYJA-UHFFFAOYSA-N
Formula:	C13H11Br
SMILES:	BrC(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	247.13
CAS:	776-74-9

Physical Properties

Property code	Value	Unit	Source
gf	295.28	kJ/mol	Joback Method
hf	182.46	kJ/mol	Joback Method
hfus	19.27	kJ/mol	Joback Method
hvap	55.13	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	4.171		Crippen Method
mcvol	164.010	ml/mol	McGowan Method
pc	3352.86	kPa	Joback Method
rinsol	1593.00		NIST Webbook
tb	615.92	K	Joback Method
tc	880.26	K	Joback Method
tf	318.00	K	NIST Webbook
vc	0.604	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	364.81	J/molxK	615.92	Joback Method
cpg	380.54	J/molxK	659.98	Joback Method
cpg	394.83	J/molxK	704.03	Joback Method
cpg	407.81	J/molxK	748.09	Joback Method
cpg	419.60	J/molxK	792.14	Joback Method
cpg	430.30	J/molxK	836.20	Joback Method
cpg	440.04	J/molxK	880.26	Joback Method
dvisc	0.0025360	Paxs	333.91	Joback Method
dvisc	0.0012456	Paxs	380.91	Joback Method
dvisc	0.0007152	Paxs	427.91	Joback Method
dvisc	0.0004583	Paxs	474.91	Joback Method
dvisc	0.0003182	Paxs	521.92	Joback Method
dvisc	0.0002347	Paxs	568.92	Joback Method
dvisc	0.0001813	Paxs	615.92	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	457.20	K	2.70	NIST Webbook
tbrp	425.70	K	0.30	NIST Webbook
tbrp	457.00	K	2.70	NIST Webbook
tbrp	425.50 ± 2.50	K	0.30	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=C776749&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
rinpola:	Non-polar retention indices
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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