1,4-Dibromo-1,4-diphenyl-butadiene

Other names: 1,3-Butadiene, 1,4-dibromo-1,4-diphenyl-
Inchi: InChI=1S/C16H12Br2/c17-15(13-7-3-1-4-8-13)11-12-16(18)14-9-5-2-6-10-14/h1-12H/b15
InchiKey: VYKJGULDTAGCMJ-NFLUSIDLSA-N
Formula: C16H12Br2
SMILES: BrC(=CC=C(Br)c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 364.07
CAS: 116862-67-0

Physical Properties

Property code	Value	Unit	Source
gf	480.64	kJ/mol	Joback Method
hf	367.01	kJ/mol	Joback Method
hfus	33.63	kJ/mol	Joback Method
hvap	68.71	kJ/mol	Joback Method
log10ws	-6.62		Crippen Method
logp	5.858		Crippen Method
mcvol	215.180	ml/mol	McGowan Method
pc	2953.69	kPa	Joback Method
tb	759.24	K	Joback Method
tc	1041.29	K	Joback Method
tf	404.44	K	Joback Method
vc	0.801	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	502.61	J/mol×K	759.24	Joback Method
cpg	516.51	J/mol×K	806.25	Joback Method
cpg	529.23	J/mol×K	853.26	Joback Method
cpg	541.04	J/mol×K	900.27	Joback Method
cpg	552.18	J/mol×K	947.28	Joback Method
cpg	562.89	J/mol×K	994.29	Joback Method
cpg	573.42	J/mol×K	1041.29	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=C116862670&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
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