

BENZENE, 1,1'-(1,3-BUTADIENYLIDENE)BIS-

Other names:	1,1-diphenyl-1,3-butadiene
Inchi:	InChI=1S/C16H14/c1-2-9-16(14-10-5-3-6-11-14)15-12-7-4-8-13-15/h2-13H,1H2
InchiKey:	GUPMCMZMDAGSPF-UHFFFAOYSA-N
Formula:	C16H14
SMILES:	C=CC=C(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	206.29

Physical Properties

Property code	Value	Unit	Source
hf	349.45	kJ/mol	Cheméo Relay (1.0)
hfus	22.89	kJ/mol	Joback Method
hvap	75.34	kJ/mol	Cheméo Relay (1.0)
ie	7.83	eV	Cheméo Relay (1.0)
logp	4.304		Crippen Method
mcvol	180.180	ml/mol	McGowan Method
pc	2517.59	kPa	Joback Method
tb	582.35	K	Cheméo Relay (1.0)
tc	816.82	K	Cheméo Relay (1.0)
tf	317.72	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.75	J/mol×K	619.56	Joback Method
cpg	447.56	J/mol×K	661.24	Joback Method
cpg	463.88	J/mol×K	702.93	Joback Method
cpg	478.84	J/mol×K	744.61	Joback Method
cpg	492.57	J/mol×K	786.30	Joback Method
cpg	505.19	J/mol×K	827.98	Joback Method
cpg	516.83	J/mol×K	869.66	Joback Method

Sources

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=C4165815&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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

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