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

Inchi: InChI=1S/C16H16/c1-2-9-16(14-10-5-3-6-11-14)15-12-7-4-8-13-15/h3-13H,2H2,1H3
InchiKey: FKDKAGHZAOFATR-UHFFFAOYSA-N
Formula: C16H16
SMILES: CCC=C(c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 208.30
CAS: 1726-14-3

Physical Properties

Property code	Value	Unit	Source
gf	380.33	kJ/mol	Joback Method
hf	206.92	kJ/mol	Joback Method
hfus	24.17	kJ/mol	Joback Method
hvap	55.80	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	4.528		Crippen Method
mcvol	184.480	ml/mol	McGowan Method
pc	2414.74	kPa	Joback Method
tb	567.90 ± 0.60	K	NIST Webbook
tc	867.49	K	Joback Method
tf	271.96 ± 0.20	K	NIST Webbook
vc	0.697	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.37	J/mol×K	622.88	Joback Method
cpg	469.82	J/mol×K	663.65	Joback Method
cpg	486.81	J/mol×K	704.42	Joback Method
cpg	502.47	J/mol×K	745.19	Joback Method
cpg	516.88	J/mol×K	785.96	Joback Method
cpg	530.18	J/mol×K	826.73	Joback Method
cpg	542.48	J/mol×K	867.49	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1726143&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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