

Benzene, 1,1',1'',1'''-(1-ethanyl-2-ylidyne)tetrakis-

Other names: Benzene, 1,1',1'',1'''-(1-ethanyl-2-ylidyne)tetrakis-
Ethane, 1,1,1,2-tetraphenyl-

Inchi: InChI=1S/C26H22/c1-5-13-22(14-6-1)21-26(23-15-7-2-8-16-23,24-17-9-3-10-18-24)25-19

InchiKey: KGSFMPRFQVLGTJ-UHFFFAOYSA-N

Formula: C26H22

SMILES: c1ccc(CC(c2ccccc2)(c2ccccc2)c2ccccc2)cc1

Mol. weight [g/mol]: 334.46

Physical Properties

Property code	Value	Unit	Source
af	0.5650		Cheméo Relay (1.0)
chs	-13401.10 ± 1.30	kJ/mol	NIST Webbook
chs	-13606.00 ± 3.00	kJ/mol	NIST Webbook
hf	365.00 ± 3.00	kJ/mol	NIST Webbook
hfs	233.00 ± 3.00	kJ/mol	NIST Webbook
hfus	31.85	kJ/mol	Joback Method
hsub	132.60 ± 2.10	kJ/mol	NIST Webbook
hsub	132.00	kJ/mol	NIST Webbook
hsub	133.00	kJ/mol	NIST Webbook
hvap	111.30	kJ/mol	Cheméo Relay (1.0)
ie	8.25	eV	Cheméo Relay (1.0)
log10ws	-7.50		Cheméo Relay (1.0)
logp	6.264		Crippen Method
mcvol	282.160	ml/mol	McGowan Method
pc	1778.84	kPa	Joback Method
tb	688.70	K	Cheméo Relay (1.0)
tc	1012.17	K	Cheméo Relay (1.0)
tf	414.25 ± 0.50	K	NIST Webbook
tf	416.75 ± 0.30	K	NIST Webbook
tf	414.25 ± 0.50	K	NIST Webbook
tf	416.75 ± 0.30	K	NIST Webbook
tf	417.00 ± 2.00	K	NIST Webbook
vc	1.004	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	851.41	J/mol×K	897.77	Joback Method
cpg	940.52	J/mol×K	1179.33	Joback Method
cpg	927.56	J/mol×K	1132.41	Joback Method
cpg	914.23	J/mol×K	1085.48	Joback Method
cpg	900.25	J/mol×K	1038.55	Joback Method
cpg	885.31	J/mol×K	991.62	Joback Method
cpg	869.13	J/mol×K	944.70	Joback Method
cps	395.40	J/mol×K	298.50	NIST Webbook
dvisc	0.0000703	Pa×s	762.14	Joback Method
dvisc	0.0000378	Pa×s	897.77	Joback Method
dvisc	0.0000502	Pa×s	829.95	Joback Method
dvisc	0.0006814	Pa×s	490.88	Joback Method
dvisc	0.0001050	Pa×s	694.33	Joback Method
dvisc	0.0001711	Pa×s	626.51	Joback Method
dvisc	0.0003140	Pa×s	558.69	Joback Method
hsubt	128.70 ± 2.10	kJ/mol	370.00	NIST Webbook
hsubt	126.40 ± 1.70	kJ/mol	434.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	551.70	K	2.80	NIST Webbook

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=C2294942&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

af:	Acentric Factor
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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