Tricyclo[8.2.2.2(4,7)]hexadeca-2,4,6,8,10,12,13,15-

Other names: [2.2]-Paracyclophane-1,9-diene
Inchi: InChI=1S/C16H12/c1-2-14-4-3-13(1)9-10-15-5-7-16(8-6-15)12-11-14/h1-12H/b10-9-,12-1
InchiKey: YLCDUOJDMCMBJY-YFDRDTFESA-N
Formula: C16H12
SMILES: C1=Cc2ccc(cc2)C=Cc2ccc1cc2
Mol. weight [g/mol]: 204.27
CAS: 6572-60-7

Physical Properties

Property code	Value	Unit	Source
gf	405.68	kJ/mol	Joback Method
hf	279.09	kJ/mol	Joback Method
hfus	21.91	kJ/mol	Joback Method
hsub	93.10 ± 1.20	kJ/mol	NIST Webbook
hvap	58.06	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.341		Crippen Method
mcvol	169.320	ml/mol	McGowan Method
pc	2884.30	kPa	Joback Method
tb	642.80	K	Joback Method
tc	905.43	K	Joback Method
tf	368.14	K	Joback Method
vc	0.637	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	412.52	J/mol×K	642.80	Joback Method
cpg	429.21	J/mol×K	686.57	Joback Method
cpg	444.42	J/mol×K	730.34	Joback Method
cpg	458.29	J/mol×K	774.11	Joback Method
cpg	470.95	J/mol×K	817.88	Joback Method
cpg	482.55	J/mol×K	861.65	Joback Method
cpg	493.25	J/mol×K	905.43	Joback Method

dvisc	0.0009586	Pa×s	413.92	Joback Method
dvisc	0.0015202	Pa×s	368.14	Joback Method
dvisc	0.0006626	Pa×s	459.69	Joback Method
dvisc	0.0004897	Pa×s	505.47	Joback Method
dvisc	0.0003805	Pa×s	551.25	Joback Method
dvisc	0.0003074	Pa×s	597.02	Joback Method
dvisc	0.0002560	Pa×s	642.80	Joback Method
hfust	30.71	kJ/mol	505.90	NIST Webbook
hsubt	92.00 ± 1.20	kJ/mol	330.50	NIST Webbook

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=C6572607&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hfust: Enthalpy of fusion at a given temperature
hsub: Enthalpy of sublimation at standard conditions
hsubt: Enthalpy of sublimation at a given temperature
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