5,16:8,13-Diethenodibenzo[a,g]cyclododecane, 6,7,14,15-tetrahydro

Other names: anti-(5,16:8,13)-Diethenodibenzo[a,g] cyclododecene 6,7,14,15-tetrahydro-[2,2]-(1,4)-Naphthalenophane

Inchi: InChI=1S/C24H24/c1-2-6-22-18-10-9-17(21(22)5-1)13-14-19-11-12-20(16-15-18)24-8-4-3

InchiKey: YWFIZNFETZCKEP-FIWHBWSRSA-N

Formula: C24H20

SMILES: c1ccc2c(c1)C1CCc3ccc(c4ccccc34)CCC2CC1

Mol. weight [g/mol]: 308.42

CAS: 17341-02-5

Physical Properties

Property code	Value	Unit	Source
gf	551.08	kJ/mol	Joback Method
hf	224.31	kJ/mol	Joback Method
hfus	33.92	kJ/mol	Joback Method
hvap	77.37	kJ/mol	Joback Method
ie	7.30	eV	NIST Webbook
ie	7.50	eV	NIST Webbook
log10ws	-7.85		Crippen Method
logp	6.380		Crippen Method
mcvol	260.320	ml/mol	McGowan Method
pc	1810.77	kPa	Joback Method
tb	857.82	K	Joback Method
tc	1123.14	K	Joback Method
tf	512.18	K	Joback Method
vc	0.984	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	823.37	J/mol×K	857.82	Joback Method
cpg	843.52	J/mol×K	902.04	Joback Method
cpg	862.29	J/mol×K	946.26	Joback Method
cpg	879.92	J/mol×K	990.48	Joback Method
cpg	896.65	J/mol×K	1034.70	Joback Method

cpg	912.74	J/mol×K	1078.92	Joback Method
cpg	928.41	J/mol×K	1123.14	Joback Method
dvisc	0.0020192	Pa×s	512.18	Joback Method
dvisc	0.0014780	Pa×s	569.79	Joback Method
dvisc	0.0011456	Pa×s	627.39	Joback Method
dvisc	0.0009268	Pa×s	685.00	Joback Method
dvisc	0.0007749	Pa×s	742.61	Joback Method
dvisc	0.0006648	Pa×s	800.21	Joback Method
dvisc	0.0005822	Pa×s	857.82	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C17341025&Units=SI

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
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
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume