Anti tricyclo[4.2.2.2(2,5)]dodeca-3,7-diene

Inchi: InChI=1S/C12H16/c1-2-10-4-3-9(1)11-5-7-12(10)8-6-11/h1-2,5,7,9-12H,3-4,6,8H2/t9-,10-
InchiKey: YPRIZWMBCSCOSH-DDHJBXDOSA-N
Formula: C12H16
SMILES: C1=CC2CCC1C1C=CC2CC1
Mol. weight [g/mol]: 160.26
CAS: 69349-54-8

Physical Properties

Property code	Value	Unit	Source
gf	248.32	kJ/mol	Joback Method
hf	143.00	kJ/mol	NIST Webbook
hfus	18.46	kJ/mol	Joback Method
hvap	42.84	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	3.165		Crippen Method
mcvol	138.760	ml/mol	McGowan Method
pc	2871.95	kPa	Joback Method
tb	500.64	K	Joback Method
tc	729.20	K	Joback Method
tf	265.54	K	Joback Method
vc	0.525	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.98	J/mol×K	500.64	Joback Method
cpg	356.96	J/mol×K	538.73	Joback Method
cpg	377.33	J/mol×K	576.83	Joback Method
cpg	396.21	J/mol×K	614.92	Joback Method
cpg	413.70	J/mol×K	653.02	Joback Method
cpg	429.90	J/mol×K	691.11	Joback Method
cpg	444.92	J/mol×K	729.20	Joback Method
dvisc	0.0011498	Pa×s	265.54	Joback Method
dvisc	0.0010988	Pa×s	304.72	Joback Method

dvisc	0.0010609	Pa×s	343.91	Joback Method
dvisc	0.0010317	Pa×s	383.09	Joback Method
dvisc	0.0010086	Pa×s	422.27	Joback Method
dvisc	0.0009897	Pa×s	461.46	Joback Method
dvisc	0.0009741	Pa×s	500.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C69349548&Units=SI
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

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
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

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