

trans (cis,cis)-Bicyclo[10.1.0]trideca-4,8-diene

Inchi:	InChI=1S/C12H18/c1-2-4-6-8-11-10-12(11)9-7-5-3-1/h2,4-5,7,11-12H,1,3,6,8-10H2/b4-2
InchiKey:	XCVZOUWBCYZZSQ-ILNZVKDWSA-N
Formula:	C12H18
SMILES:	C1=C\CCC2CC2C/C=C\CC/1
Mol. weight [g/mol]:	162.28

Physical Properties

Property code	Value	Unit	Source
hf	113.25	kJ/mol	Cheméo Relay (1.0)
hfus	12.95	kJ/mol	Joback Method
hvap	63.10	kJ/mol	Cheméo Relay (1.0)
ie	8.55	eV	Cheméo Relay (1.0)
logp	3.699		Crippen Method
mcvol	149.620	ml/mol	McGowan Method
rinpol	1382.00		NIST Webbook
rinpol	1382.00		NIST Webbook
tb	502.24	K	Cheméo Relay (1.0)
tf	283.40	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.94	J/mol×K	511.38	Joback Method
cpg	469.20	J/mol×K	748.33	Joback Method
cpg	452.85	J/mol×K	708.84	Joback Method
cpg	435.17	J/mol×K	669.35	Joback Method
cpg	416.09	J/mol×K	629.85	Joback Method
cpg	395.57	J/mol×K	590.36	Joback Method
cpg	373.54	J/mol×K	550.87	Joback Method
dvisc	0.0007261	Pa×s	376.33	Joback Method
dvisc	0.0002539	Pa×s	511.38	Joback Method
dvisc	0.0003368	Pa×s	466.36	Joback Method
dvisc	0.0004747	Pa×s	421.35	Joback Method
dvisc	0.0067331	Pa×s	241.28	Joback Method

dvisc	0.0012468	Pa×s	331.31	Joback Method
dvisc	0.0025376	Pa×s	286.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R2854&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
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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