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

Inchi: InChI=1S/C13H20/c1-2-4-6-8-10-13-11-12(13)9-7-5-3-1/h3-6,12-13H,1-2,7-11H2/b5-3+,6
InchiKey: OKQPAVLKCLUCOF-KSNBDJSYSA-N
Formula: C13H20
SMILES: C1=CCCC2CC2CCC=CCC1
Mol. weight [g/mol]: 176.30

Physical Properties

Property code	Value	Unit	Source
gf	155.30	kJ/mol	Joback Method
hf	-93.61	kJ/mol	Joback Method
hfus	13.44	kJ/mol	Joback Method
hvap	46.15	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	4.089		Crippen Method
mcvol	163.710	ml/mol	McGowan Method
pc	2605.74	kPa	Joback Method
rinpol	1357.00		NIST Webbook
tb	538.53	K	Joback Method
tc	779.84	K	Joback Method
tf	249.03	K	Joback Method
vc	0.594	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.16	J/mol×K	538.53	Joback Method
cpg	426.48	J/mol×K	578.75	Joback Method
cpg	450.08	J/mol×K	618.97	Joback Method
cpg	472.03	J/mol×K	659.18	Joback Method
cpg	492.38	J/mol×K	699.40	Joback Method
cpg	511.18	J/mol×K	739.62	Joback Method
cpg	528.50	J/mol×K	779.84	Joback Method
dvisc	0.0093345	Pa×s	249.03	Joback Method
dvisc	0.0028788	Pa×s	297.28	Joback Method

dvisc	0.0012331	Pa×s	345.53	Joback Method
dvisc	0.0006502	Pa×s	393.78	Joback Method
dvisc	0.0003942	Pa×s	442.03	Joback Method
dvisc	0.0002638	Pa×s	490.28	Joback Method
dvisc	0.0001897	Pa×s	538.53	Joback Method

Sources

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=R2778&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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