trans-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/h3,5-6,8,12-13H,1-2,4,7,9-11H2/
InchiKey: GHHBBIQEXATKDO-QFXXITGJSA-N
Formula: C13H20
SMILES: C1=C/CCC2CC2C/C=C/CCC/1
Mol. weight [g/mol]: 176.30

Physical Properties

Property code	Value	Unit	Source
af	0.2268		Cheméo Relay (1.0)
gf	155.30	kJ/mol	Joback Method
hf	56.36	kJ/mol	Cheméo Relay (1.0)
hfus	13.44	kJ/mol	Joback Method
hvap	65.98	kJ/mol	Cheméo Relay (1.0)
ie	8.47	eV	Cheméo Relay (1.0)
log10ws	-5.17		Cheméo Relay (1.0)
logp	4.089		Crippen Method
mcvol	163.710	ml/mol	McGowan Method
pc	2605.74	kPa	Joback Method
rinpol	1398.00		NIST Webbook
tb	526.52	K	Cheméo Relay (1.0)
tc	733.02	K	Cheméo Relay (1.0)
tf	299.89	K	Cheméo Relay (1.0)
vc	0.524	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

dvisc	0.0006502	Pa×s	393.78	Joback Method
dvisc	0.0001897	Pa×s	538.53	Joback Method
dvisc	0.0002638	Pa×s	490.28	Joback Method
dvisc	0.0003942	Pa×s	442.03	Joback Method
dvisc	0.0093345	Pa×s	249.03	Joback Method
dvisc	0.0012331	Pa×s	345.53	Joback Method
dvisc	0.0028788	Pa×s	297.28	Joback Method

Sources

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.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R2663&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
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
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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