

1-Ethenyl-1-methyl-2,4-bis-(1-methylethenyl)-1S-1

Inchi:

InChI=1S/C2H6/c1-2/h1-2H3

InchiKey:

OTMSDBZUPAUEDD-UHFFFAOYSA-N

Formula:

C2H6

SMILES:

CC

Mol. weight [g/mol]:

30.07

Physical Properties

Property code	Value	Unit	Source
af	0.1482		Cheméo Relay (1.0)
gf	-34.04	kJ/mol	Joback Method
hf	-59.43	kJ/mol	Cheméo Relay (1.0)
hfus	0.94	kJ/mol	Joback Method
hvap	10.33	kJ/mol	Cheméo Relay (1.0)
ie	11.24	eV	Cheméo Relay (1.0)
log10ws	-1.50		Cheméo Relay (1.0)
logp	1.026		Crippen Method
mcvol	39.040	ml/mol	McGowan Method
pc	5029.93	kPa	Joback Method
ripol	1580.00		NIST Webbook
tb	188.07	K	Cheméo Relay (1.0)
tc	297.51	K	Cheméo Relay (1.0)
tf	84.11	K	Cheméo Relay (1.0)
vc	0.150	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	43.67	J/mol×K	245.16	Joback Method
cpg	66.03	J/mol×K	401.63	Joback Method
cpg	62.55	J/mol×K	375.55	Joback Method
cpg	58.97	J/mol×K	349.47	Joback Method
cpg	55.29	J/mol×K	323.39	Joback Method
cpg	51.52	J/mol×K	297.32	Joback Method
cpg	47.64	J/mol×K	271.24	Joback Method

dvisc	0.0002148	Pa×s	178.73	Joback Method
dvisc	0.0001008	Pa×s	245.16	Joback Method
dvisc	0.0001234	Pa×s	223.02	Joback Method
dvisc	0.0001579	Pa×s	200.87	Joback Method
dvisc	0.0011192	Pa×s	112.30	Joback Method
dvisc	0.0003187	Pa×s	156.59	Joback Method
dvisc	0.0005385	Pa×s	134.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R633468&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.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

<https://www.chemeo.com/cid/71-444-0/1-Ethenyl-1-methyl-2-4-bis-1-methylethenyl-1S-1-alpha-2-beta-4-alpha-cyclohexyl>

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