

(E,E)-1,6-Cyclodecadiene, 4-methyl

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C13H22/c1-13-11-9-7-5-3-2-4-6-8-10-12-13/h7-10,13H,2-6,11-12H2,1H3/b9-7+

LCRODOUAEKFGHL-FIFLTTTCUSA-N

C13H22

CC1CC=CCCCCCC=CC1

178.31

Physical Properties

Property code	Value	Unit	Source
gf	70.35	kJ/mol	Joback Method
hf	-178.73	kJ/mol	Joback Method
hfus	11.10	kJ/mol	Joback Method
hvap	46.58	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	4.479		Crippen Method
mcvol	174.570	ml/mol	McGowan Method
pc	2405.28	kPa	Joback Method
rinpol	1150.00		NIST Webbook
tb	540.33	K	Joback Method
tc	780.92	K	Joback Method
tf	224.05	K	Joback Method
vc	0.621	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	416.72	J/mol×K	540.33	Joback Method
cpg	443.11	J/mol×K	580.43	Joback Method
cpg	467.93	J/mol×K	620.53	Joback Method
cpg	491.15	J/mol×K	660.62	Joback Method
cpg	512.79	J/mol×K	700.72	Joback Method
cpg	532.81	J/mol×K	740.82	Joback Method
cpg	551.23	J/mol×K	780.92	Joback Method
dvisc	0.0729791	Pa×s	224.05	Joback Method
dvisc	0.0070607	Pa×s	276.76	Joback Method

dvisc	0.0014424	Pa×s	329.48	Joback Method
dvisc	0.0004566	Pa×s	382.19	Joback Method
dvisc	0.0001911	Pa×s	434.90	Joback Method
dvisc	0.0000965	Pa×s	487.62	Joback Method
dvisc	0.0000557	Pa×s	540.33	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R2749&Units=SI

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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