Cyclohexene, 6-(2-butenyl)-1,5,5-trimethyl-, (E)-

Inchi: InChI=1S/C13H22/c1-5-6-9-12-11(2)8-7-10-13(12,3)4/h5-6,8,12H,7,9-10H2,1-4H3/b6-5-

InchiKey: SNHNEPFADCCPAL-WAYWQWQTSA-N

Formula: C13H22

SMILES: CC=CCC1C(C)=CCCC1(C)C

Mol. weight [g/mol]: 178.31

CAS: 53941-16-5

Physical Properties

Property code	Value	Unit	Source
gf	170.38	kJ/mol	Joback Method
hf	-98.90	kJ/mol	Joback Method
hfus	17.07	kJ/mol	Joback Method
hvap	44.41	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	4.335		Crippen Method
mcvol	174.570	ml/mol	McGowan Method
pc	2111.94	kPa	Joback Method
ripol	2027.00		NIST Webbook
ripol	2027.00		NIST Webbook
tb	520.26	K	Joback Method
tc	729.88	K	Joback Method
tf	271.51	K	Joback Method
vc	0.659	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	411.92	J/mol×K	520.26	Joback Method
cpg	432.23	J/mol×K	555.20	Joback Method
cpg	451.33	J/mol×K	590.13	Joback Method
cpg	469.33	J/mol×K	625.07	Joback Method
cpg	486.35	J/mol×K	660.01	Joback Method
cpg	502.50	J/mol×K	694.95	Joback Method
cpg	517.90	J/mol×K	729.88	Joback Method

Sources

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=C53941165&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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