Acora-2,4-diene

Other names: Acora-3,5-diene
Inchi: InChI=1S/C15H24/c1-11(2)14-6-5-13(4)15(14)9-7-12(3)8-10-15/h7-9,11,13-14H,5-6,10H
InchiKey: ZQMYLSWMANINAL-QLFBSQMISA-N
Formula: C15H24
SMILES: CC1=CCC2(C=C1)C(C)CCC2C(C)C
Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
gf	183.17	kJ/mol	Joback Method
hf	-138.26	kJ/mol	Joback Method
hfus	15.78	kJ/mol	Joback Method
hvap	48.90	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	4.581		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	2027.23	kPa	Joback Method
rinpol	1421.00		NIST Webbook
rinpol	1421.00		NIST Webbook
ripol	1601.00		NIST Webbook
tb	571.59	K	Joback Method
tc	794.61	K	Joback Method
tf	299.31	K	Joback Method
vc	0.721	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.14	J/mol×K	571.59	Joback Method
cpg	524.19	J/mol×K	608.76	Joback Method
cpg	545.79	J/mol×K	645.93	Joback Method
cpg	566.10	J/mol×K	683.10	Joback Method
cpg	585.27	J/mol×K	720.27	Joback Method
cpg	603.45	J/mol×K	757.44	Joback Method

cpg	620.81	J/mol×K	794.61	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=R198886&Units=SI

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