(R)-2-Methyl-5-(6-methylhepta-1,5-dien-2-yl)cyclo

Inchi: InChI=1S/C15H22O/c1-11(2)6-5-7-12(3)14-9-8-13(4)15(16)10-14/h6,8,14H,3,5,7,9-10H2
InchiKey: FNSXIWZZZIJORF-AWEZNQCLSA-N
Formula: C15H22O
SMILES: C=C(CCC=C(C)C)C1CC=C(C)C(=O)C1
Mol. weight [g/mol]: 218.33
CAS: 5988-72-7

Physical Properties

Property code	Value	Unit	Source
gf	148.57	kJ/mol	Joback Method
hf	-166.93	kJ/mol	Joback Method
hfus	23.09	kJ/mol	Joback Method
hvap	54.06	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.214		Crippen Method
mcvol	200.020	ml/mol	McGowan Method
pc	1901.92	kPa	Joback Method
rinpol	1734.10		NIST Webbook
rinpol	1734.10		NIST Webbook
rinpol	1725.00		NIST Webbook
rinpol	1725.00		NIST Webbook
tb	634.71	K	Joback Method
tc	854.27	K	Joback Method
tf	312.93	K	Joback Method
vc	0.764	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	532.11	J/mol×K	634.71	Joback Method
cpg	552.12	J/mol×K	671.30	Joback Method
cpg	570.96	J/mol×K	707.90	Joback Method
cpg	588.67	J/mol×K	744.49	Joback Method
cpg	605.27	J/mol×K	781.08	Joback Method

cpg	620.81	J/mol×K	817.68	Joback Method
cpg	635.31	J/mol×K	854.27	Joback Method

Sources

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=C5988727&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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