(E)-4-((1R,5S)-2,5,6,6-Tetramethylcyclohex-2-en-1-

Inchi: InChI=1S/C14H22O/c1-10-6-7-11(2)14(4,5)13(10)9-8-12(3)15/h6,8-9,11,13H,7H2,1-5H3/
InchiKey: JZQOJFLIJNRDHK-CMDGGOBGSA-N
Formula: C14H22O
SMILES: CC(=O)C=CC1C(C)=CCC(C)C1(C)C
Mol. weight [g/mol]: 206.32
CAS: 472-46-8

Physical Properties

Property code	Value	Unit	Source
gf	42.17	kJ/mol	Joback Method
hf	-252.46	kJ/mol	Joback Method
hfus	22.33	kJ/mol	Joback Method
hvap	53.08	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	3.760		Crippen Method
mcvol	190.230	ml/mol	McGowan Method
pc	1989.43	kPa	Joback Method
rinpol	1545.90		NIST Webbook
rinpol	1545.90		NIST Webbook
tb	592.34	K	Joback Method
tc	806.59	K	Joback Method
tf	328.47	K	Joback Method
vc	0.721	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	490.54	J/mol×K	592.34	Joback Method
cpg	510.15	J/mol×K	628.05	Joback Method
cpg	528.68	J/mol×K	663.76	Joback Method
cpg	546.23	J/mol×K	699.46	Joback Method
cpg	562.93	J/mol×K	735.17	Joback Method
cpg	578.89	J/mol×K	770.88	Joback Method
cpg	594.23	J/mol×K	806.59	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=C472468&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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