E-7-isopropenyl-4-methyl-10-methylene-4-cyclode

Inchi: InChI=1S/C15H22O/c1-11(2)14-8-5-12(3)6-10-15(16)13(4)7-9-14/h5,14H,1,4,6-10H2,2-3
InchiKey: QMEZKUJMSSOSEF-LFYBBSHMSA-N
Formula: C15H22O
SMILES: C=C1CCC(C(=C)C)CC=C(C)CCC1=O
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	81.58	kJ/mol	Joback Method
hf	-214.76	kJ/mol	Joback Method
hfus	14.63	kJ/mol	Joback Method
hvap	54.87	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.214		Crippen Method
mcvol	200.020	ml/mol	McGowan Method
pc	2009.10	kPa	Joback Method
rinpol	1665.00		NIST Webbook
rinpol	1665.00		NIST Webbook
tb	646.91	K	Joback Method
tc	884.73	K	Joback Method
tf	331.57	K	Joback Method
vc	0.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.64	J/mol×K	646.91	Joback Method
cpg	562.65	J/mol×K	686.55	Joback Method
cpg	584.17	J/mol×K	726.18	Joback Method
cpg	604.16	J/mol×K	765.82	Joback Method
cpg	622.60	J/mol×K	805.46	Joback Method
cpg	639.45	J/mol×K	845.10	Joback Method
cpg	654.69	J/mol×K	884.73	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=R513072&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume