3,7-Cyclodecadien-1-one, 3,7-dimethyl-10-(1-methylethylidene)-, (E,E)-

Other names: Germacra-3,7(11),9-trien-6-one, (E,E)-
Germacron
Germacrone
3,7-Dimethyl-10-(1-methylethylidene)-3,7-cyclodecadien-1-one, (trans,trans)-
(E,E)-Germacrone

Inchi: InChI=1S/C15H22O/c1-11(2)14-9-8-12(3)6-5-7-13(4)10-15(14)16/h7-8H,5-6,9-10H2,1-4H

InchiKey: CAULGCQHVOVVRN-SVGXSMIJSA-N

Formula: C15H22O

SMILES: CC1=CCC(=C(C)C)C(=O)CC(C)=CCC1

Mol. weight [g/mol]: 218.33

CAS: 6902-91-6

Physical Properties

Property code	Value	Unit	Source
gf	14.16	kJ/mol	Joback Method
hf	-281.75	kJ/mol	Joback Method
hfus	17.16	kJ/mol	Joback Method
hvap	57.43	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	4.359		Crippen Method
mcvol	200.020	ml/mol	McGowan Method
pc	2049.31	kPa	Joback Method
rinpol	1669.00		NIST Webbook
rinpol	1696.00		NIST Webbook
rinpol	1693.00		NIST Webbook
rinpol	1689.00		NIST Webbook
rinpol	1693.00		NIST Webbook
rinpol	1707.90		NIST Webbook
rinpol	1694.00		NIST Webbook
rinpol	1677.00		NIST Webbook
rinpol	1733.00		NIST Webbook
rinpol	1690.00		NIST Webbook
rinpol	1705.00		NIST Webbook
rinpol	1675.00		NIST Webbook
rinpol	1658.00		NIST Webbook
rinpol	1691.00		NIST Webbook
rinpol	1690.00		NIST Webbook

rinpol	1694.00		NIST Webbook
rinpol	1693.00		NIST Webbook
rinpol	1694.00		NIST Webbook
rinpol	1694.00		NIST Webbook
rinpol	1687.00		NIST Webbook
rinpol	1694.00		NIST Webbook
rinpol	1644.00		NIST Webbook
rinpol	1705.00		NIST Webbook
rinpol	1688.00		NIST Webbook
rinpol	1691.30		NIST Webbook
ripol	2212.00		NIST Webbook
ripol	2217.00		NIST Webbook
ripol	2254.00		NIST Webbook
ripol	2223.00		NIST Webbook
ripol	2209.00		NIST Webbook
tb	666.52	K	Joback Method
tc	907.31	K	Joback Method
tf	347.53	K	Joback Method
vc	0.741	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.74	J/mol×K	666.52	Joback Method
cpg	561.51	J/mol×K	706.65	Joback Method
cpg	581.83	J/mol×K	746.78	Joback Method
cpg	600.67	J/mol×K	786.92	Joback Method
cpg	618.01	J/mol×K	827.05	Joback Method
cpg	633.82	J/mol×K	867.18	Joback Method
cpg	648.08	J/mol×K	907.31	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=C6902916&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