4H-Inden-4-one, 1,2,3,5,6,7-hexahydro-1,1,2,3,3-pentamethyl-

Other names: Cashmeran
1,2,3,5,6,7-hexahydro-1,1,2,3,3-pentamethyl-4H-inden-4-one
Inchi: InChI=1S/C14H22O/c1-9-13(2,3)10-7-6-8-11(15)12(10)14(9,4)5/h9H,6-8H2,1-5H3
InchiKey: MIZGSAALSYARKU-UHFFFAOYSA-N
Formula: C14H22O
SMILES: CC1C(C)(C)C2=C(C(=O)CCC2)C1(C)C
Mol. weight [g/mol]: 206.32
CAS: 33704-61-9

Physical Properties

Property code	Value	Unit	Source
gf	21.62	kJ/mol	Joback Method
hf	-297.89	kJ/mol	Joback Method
hfus	10.41	kJ/mol	Joback Method
hvap	50.35	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.738		Crippen Method
mcvol	183.670	ml/mol	McGowan Method
pc	2206.22	kPa	Joback Method
rinpol	1503.20		NIST Webbook
rinpol	1503.20		NIST Webbook
tb	618.76	K	Joback Method
tc	854.47	K	Joback Method
tf	410.44	K	Joback Method
vc	0.698	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	504.54	J/mol×K	618.76	Joback Method
cpg	525.27	J/mol×K	658.04	Joback Method
cpg	544.99	J/mol×K	697.33	Joback Method
cpg	563.94	J/mol×K	736.61	Joback Method
cpg	582.36	J/mol×K	775.90	Joback Method

cpg	600.51	J/mol×K	815.18	Joback Method
cpg	618.62	J/mol×K	854.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33704619&Units=SI
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

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