

Cashmeran

Other names:	1,2,3,5,6,7-hexahydro-1,1,2,3,3-pentamethyl-4H-inden-4-one Cashmeran
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:	<chem>CC1C(C)(C)C2=C(C(=O)CCC2)C1(C)C</chem>
Mol. weight [g/mol]:	206.33

Physical Properties

Property code	Value	Unit	Source
hfus	10.41	kJ/mol	Joback Method
logp	3.738		Crippen Method
mcvol	183.670	ml/mol	McGowan 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

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

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

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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