TRICYCLO[5.2.1.0(2,6)]DECAN-8-ONE

Other names:	4,7-Methanoindan-5(4H)-one, tetrahydro-
	Tricyclo(5,2,1,0(2,6))decanone-8
	Tricyclo[5.2.1.0(2,6)]decan-8-one
	Corodane
	8-Ketotricyclo(5.2.1.0(sup2,6))decane
	8-Oxotricyclo(5.2.1.0(2,6))decane
	Tricyclo[5.2.1.0(2,6)]decanone-8
	NSC 77098
	4,7-Methanoindan-6-one, hexahydro
	tricyclo[5.2.1.02,6]decane-8-one
Inchi:	InChI=1S/C10H14O/c11-10-5-6-4-9(10)8-3-1-2-7(6)8/h6-9H,1-5H2
InchiKey:	OMIDXVJKZCPKEI-UHFFFAOYSA-N
Formula:	C10H14O
SMILES:	O=C1CC2CC1C1CCCC21
Mol. weight [g/mol]:	150.22

Physical Properties

Property code	Value	Unit	Source
hf	-189.14	kJ/mol	Cheméo Relay (1.0)
hfus	14.54	kJ/mol	Joback Method
ie	9.07	eV	Cheméo Relay (1.0)
logp	2.012		Crippen Method
mcvol	120.750	ml/mol	McGowan Method
tf	388.32	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.43	J/mol×K	515.84	Joback Method
cpg	330.08	J/mol×K	554.36	Joback Method
cpg	348.41	J/mol×K	592.89	Joback Method
cpg	365.50	J/mol×K	631.41	Joback Method
cpg	381.43	J/mol×K	669.93	Joback Method
cpg	396.28	J/mol×K	708.46	Joback Method

cpg	410.13	J/mol×K	746.98	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	405.20	K	4.00	NIST Webbook

Sources

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=C13380944&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg: Ideal gas heat capacity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tbrp: Boiling point at reduced pressure
tf: Normal melting (fusion) point