

6,6,8,9-tetramethyltricyclo[3.3.3.0]-undec-7-en-2-one

Inchi: InChI=1S/C15H24O/c1-10-5-7-14-8-6-12(16)15(10,14)11(2)9-13(14,3)4/h9-10,12,16H,5-
InchiKey: JAEKBEODQWGTA-UHFFFAOYSA-N
Formula: C15H24O
SMILES: CC1=CC(C)(C)C23CCC(C)C12C(O)CC3
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	85.09	kJ/mol	Joback Method
hf	-247.73	kJ/mol	Joback Method
hfus	12.98	kJ/mol	Joback Method
hvap	62.63	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	3.530		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2412.37	kPa	Joback Method
rinpol	1580.00		NIST Webbook
ripol	2109.00		NIST Webbook
tb	659.06	K	Joback Method
tc	875.19	K	Joback Method
tf	442.91	K	Joback Method
vc	0.728	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	571.00	J/mol×K	659.06	Joback Method
cpg	589.38	J/mol×K	695.08	Joback Method
cpg	607.16	J/mol×K	731.10	Joback Method
cpg	624.69	J/mol×K	767.12	Joback Method
cpg	642.32	J/mol×K	803.15	Joback Method
cpg	660.40	J/mol×K	839.17	Joback Method
cpg	679.26	J/mol×K	875.19	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=R344524&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
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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