

2,10,14-trimethyl-6-methylene-7(3-methyl-pent-4-en-3-yn-1-yl)-1,5-dioxane

Inchi:	InChI=1S/C25H44/c1-9-11-12-13-22(6)15-17-25(16-14-21(5)10-2)24(8)19-23(7)18-20(3)
InchiKey:	IPOCVVGOCVIAHD-MLBLMHQHSA-N
Formula:	C25H44
SMILES:	<chem>C=CC(C)CCC(CC=C(C)CCC=CC)C(C)CC(=C)CC(C)C</chem>
Mol. weight [g/mol]:	344.62

Physical Properties

Property code	Value	Unit	Source
gf	468.88	kJ/mol	Joback Method
hf	-114.73	kJ/mol	Joback Method
hfus	41.64	kJ/mol	Joback Method
hvap	68.43	kJ/mol	Joback Method
log10ws	-8.74		Crippen Method
logp	8.526		Crippen Method
mcvol	345.910	ml/mol	McGowan Method
pc	871.19	kPa	Joback Method
rinpol	2144.00		NIST Webbook
tb	771.08	K	Joback Method
tc	956.29	K	Joback Method
tf	269.91	K	Joback Method
vc	1.335	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1051.81	J/mol×K	771.08	Joback Method
cpg	1073.80	J/mol×K	801.95	Joback Method
cpg	1094.71	J/mol×K	832.82	Joback Method
cpg	1114.63	J/mol×K	863.69	Joback Method
cpg	1133.62	J/mol×K	894.56	Joback Method
cpg	1151.76	J/mol×K	925.43	Joback Method
cpg	1169.13	J/mol×K	956.29	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=R394544&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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