

# (Z)-6-(2,3-dimethyltricyclo[2.2.1.0<sup>2,6</sup>]heptan-3-yl)-

<b>Inchi:</b>	InChI=1S/C16H24O/c1-10(11(2)17)6-5-7-15(3)12-8-13-14(9-12)16(13,15)4/h6,12-14H,5,
<b>InchiKey:</b>	AJAXBERBECDKTL-POHAHGRESA-N
<b>Formula:</b>	C16H24O
<b>SMILES:</b>	CC(=O)C(C)=CCCC1(C)C2CC3C(C2)C31C
<b>Mol. weight [g/mol]:</b>	232.36

## Physical Properties

Property code	Value	Unit	Source
gf	206.64	kJ/mol	Joback Method
hf	-158.20	kJ/mol	Joback Method
hfus	25.84	kJ/mol	Joback Method
hvap	54.47	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	3.984		Crippen Method
mcvol	200.990	ml/mol	McGowan Method
pc	1940.65	kPa	Joback Method
rinpol	1854.20		NIST Webbook
rinpol	1854.20		NIST Webbook
tb	626.21	K	Joback Method
tc	836.24	K	Joback Method
tf	401.15	K	Joback Method
vc	0.799	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	576.44	J/mol×K	626.21	Joback Method
cpg	595.05	J/mol×K	661.21	Joback Method
cpg	612.66	J/mol×K	696.22	Joback Method
cpg	629.56	J/mol×K	731.22	Joback Method
cpg	646.04	J/mol×K	766.23	Joback Method
cpg	662.38	J/mol×K	801.23	Joback Method
cpg	678.88	J/mol×K	836.24	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U412719&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U412719&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvp:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinp:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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