(3aR,6R,8aR)-7,7-Dimethyl-8-methylenehexahydro

Other names: Khusimone
12-nor-Zizaen-2-one
Inchi: InChI=1S/C14H20O/c1-9-11-4-5-12(15)14(11)7-6-10(8-14)13(9,2)3/h10-11H,1,4-8H2,2-3
InchiKey: BDHSOIIDXCBNPA-UCOFZHQHSA-N
Formula: C14H20O
SMILES: C=C1C2CCC(=O)C23CCC(C3)C1(C)C
Mol. weight [g/mol]: 204.31
CAS: 30557-76-7

Physical Properties

Property code	Value	Unit	Source
gf	136.85	kJ/mol	Joback Method
hf	-169.53	kJ/mol	Joback Method
hfus	9.05	kJ/mol	Joback Method
hvap	48.64	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	3.348		Crippen Method
mcvol	172.810	ml/mol	McGowan Method
pc	2472.73	kPa	Joback Method
rinpol	1604.00		NIST Webbook
rinpol	1604.00		NIST Webbook
rinpol	1605.00		NIST Webbook
rinpol	1605.00		NIST Webbook
rinpol	1605.00		NIST Webbook
tb	611.27	K	Joback Method
tc	853.73	K	Joback Method
tf	419.78	K	Joback Method
vc	0.660	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	487.80	J/mol×K	611.27	Joback Method
cpg	508.81	J/mol×K	651.68	Joback Method

cpg	528.58	J/mol×K	692.09	Joback Method
cpg	547.44	J/mol×K	732.50	Joback Method
cpg	565.72	J/mol×K	772.91	Joback Method
cpg	583.74	J/mol×K	813.32	Joback Method
cpg	601.83	J/mol×K	853.73	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C30557767&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume