(3S,3aR,6R,8aS)-7,7-Dimethyl-8-methyleneoctahyd

Other names:	1H-3a,6-Methanoazulene-3-carboxaldehyde, octahydro-7,7-dimethyl-8-methylene-, (3S,3aR,6R,8aS)- 1H-3a,6-Methanoazulene-3-carboxaldehyde, octahydro-7,7-dimethyl-8-methylene-, [3S-(3«alpha»,3a«alpha»,6«alpha»,8a«alpha»)]- Ziza[al]
Inchi:	InChI=1S/C15H22O/c1-10-13-5-4-12(9-16)15(13)7-6-11(8-15)14(10,2)3/h9,11-13H,1,4-8
InchiKey:	ONCLDGVLVUPPIN-UHFFFAOYSA-N
Formula:	C15H22O
SMILES:	C=C1C2CCC(C=O)C23CCC(C3)C1(C)C
Mol. weight [g/mol]:	218.33
CAS:	82509-29-3

Physical Properties

Property code	Value	Unit	Source
gf	160.63	kJ/mol	Joback Method
hf	-158.39	kJ/mol	Joback Method
hfus	15.49	kJ/mol	Joback Method
hvap	53.03	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.594		Crippen Method
mcvol	186.900	ml/mol	McGowan Method
pc	2265.42	kPa	Joback Method
rinpol	1680.00		NIST Webbook
rinpol	1689.00		NIST Webbook
rinpol	1691.00		NIST Webbook
rinpol	1680.00		NIST Webbook
rinpol	1663.00		NIST Webbook
rinpol	1649.00		NIST Webbook
rinpol	1645.00		NIST Webbook
tb	610.32	K	Joback Method
tc	836.85	K	Joback Method
tf	400.59	K	Joback Method
vc	0.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	529.85	J/mol×K	610.32	Joback Method
cpg	550.56	J/mol×K	648.07	Joback Method
cpg	570.01	J/mol×K	685.83	Joback Method
cpg	588.51	J/mol×K	723.58	Joback Method
cpg	606.35	J/mol×K	761.34	Joback Method
cpg	623.83	J/mol×K	799.09	Joback Method
cpg	641.24	J/mol×K	836.85	Joback Method

Sources

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=C82509293&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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