

2(1H)-Naphthalenone, octahydro-8a-methyl-, trans-

Other names:	9«beta»-Methyl-2-decalone trans-10-Methyl-2-decalone
Inchi:	InChI=1S/C11H18O/c1-11-7-3-2-4-9(11)5-6-10(12)8-11/h9H,2-8H2,1H3
InchiKey:	IDMWZWSMOJZNAC-UHFFFAOYSA-N
Formula:	C11H18O
SMILES:	CC12CCCCC1CCC(=O)C2
Mol. weight [g/mol]:	166.26
CAS:	1197-95-1

Physical Properties

Property code	Value	Unit	Source
gf	-13.24	kJ/mol	Joback Method
hf	-271.87	kJ/mol	Joback Method
hfus	5.33	kJ/mol	Joback Method
hvap	43.69	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	2.936		Crippen Method
mvol	145.700	ml/mol	McGowan Method
pc	2973.04	kPa	Joback Method
rinpol	1368.00		NIST Webbook
tb	549.70	K	Joback Method
tc	794.62	K	Joback Method
tf	327.65	K	Joback Method
vc	0.538	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.54	J/molxK	549.70	Joback Method
cpg	395.39	J/molxK	590.52	Joback Method
cpg	415.78	J/molxK	631.34	Joback Method
cpg	434.87	J/molxK	672.16	Joback Method
cpg	452.81	J/molxK	712.98	Joback Method
cpg	469.77	J/molxK	753.80	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=C1197951&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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