

(R)-(-)-4,4a,5,6,7,8-Hexahydro-4a-methyl-2(3H)-naphthalinone

Other names:	R-(-)-4,4a,5,6,7,8-Hexahydro-4a-methyl-2(3H)-naphthalinone (R)-(-)-10-Methyl-1(9)-octal-2-one
Inchi:	InChI=1S/C11H16O/c1-11-6-3-2-4-9(11)8-10(12)5-7-11/h8H,2-7H2,1H3/t11-/m0/s1
InchiKey:	OHERZLWVBJCXOF-NSHDSACASA-N
Formula:	C11H16O
SMILES:	CC12CCCCC1=CC(=O)CC2
Mol. weight [g/mol]:	164.24
CAS:	63975-59-7

Physical Properties

Property code	Value	Unit	Source
gf	14.80	kJ/mol	Joback Method
hf	-205.22	kJ/mol	Joback Method
hfus	5.09	kJ/mol	Joback Method
hvap	44.95	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	2.856		Crippen Method
mvol	141.400	ml/mol	McGowan Method
pc	3156.17	kPa	Joback Method
tb	558.51	K	Joback Method
tc	807.11	K	Joback Method
tf	345.17	K	Joback Method
vc	0.525	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.72	J/mol×K	558.51	Joback Method
cpg	373.36	J/mol×K	599.94	Joback Method
cpg	391.65	J/mol×K	641.38	Joback Method
cpg	408.77	J/mol×K	682.81	Joback Method
cpg	424.89	J/mol×K	724.24	Joback Method
cpg	440.18	J/mol×K	765.68	Joback Method
cpg	454.79	J/mol×K	807.11	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	428.20	K	2.30	NIST Webbook

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=C63975597&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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