

2«alpha»-acetoxy-trans-decalin

Inchi:	InChI=1S/C12H20O2/c1-9(13)14-12-7-6-10-4-2-3-5-11(10)8-12/h10-12H,2-8H2,1H3/t10?
InchiKey:	XKCLIFLFEJJSOAT-MCIGGMRASA-N
Formula:	C12H20O2
SMILES:	CC(=O)OC1CCC2CCCCC2C1
Mol. weight [g/mol]:	196.29

Physical Properties

Property code	Value	Unit	Source
gf	-118.37	kJ/mol	Joback Method
hf	-435.19	kJ/mol	Joback Method
hfus	18.56	kJ/mol	Joback Method
hvap	51.67	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	2.908		Crippen Method
mvol	165.660	ml/mol	McGowan Method
pc	2507.52	kPa	Joback Method
rinpol	1405.00		NIST Webbook
ripol	1864.00		NIST Webbook
tb	576.14	K	Joback Method
tc	797.36	K	Joback Method
tf	314.72	K	Joback Method
vc	0.613	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.50	J/molxK	576.14	Joback Method
cpg	465.05	J/molxK	613.01	Joback Method
cpg	485.29	J/molxK	649.88	Joback Method
cpg	504.26	J/molxK	686.75	Joback Method
cpg	522.00	J/molxK	723.62	Joback Method
cpg	538.53	J/molxK	760.49	Joback Method
cpg	553.90	J/molxK	797.36	Joback Method
dvisc	0.0029771	Paxs	314.72	Joback Method

dvisc	0.0017448	Paxs	358.29	Joback Method
dvisc	0.0011482	Paxs	401.86	Joback Method
dvisc	0.0008201	Paxs	445.43	Joback Method
dvisc	0.0006219	Paxs	489.00	Joback Method
dvisc	0.0004935	Paxs	532.57	Joback Method
dvisc	0.0004055	Paxs	576.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R136026&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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