2«alpha»-acetyloxy-trans-decalin-6-one

Inchi: InChI=1S/C12H18O3/c1-8(13)15-12-5-3-9-6-11(14)4-2-10(9)7-12/h9-10,12H,2-7H2,1H3/
InchiKey: DAQCRVQCGFADLY-CBINBANVSA-N
Formula: C12H18O3
SMILES: CC(=O)OC1CCC2CC(=O)CCC2C1
Mol. weight [g/mol]: 210.27

Physical Properties

Property code	Value	Unit	Source
gf	-240.96	kJ/mol	Joback Method
hf	-572.89	kJ/mol	Joback Method
hfus	18.07	kJ/mol	Joback Method
hvap	55.91	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	2.087		Crippen Method
mcvol	167.230	ml/mol	McGowan Method
pc	2597.78	kPa	Joback Method
rinpol	1617.00		NIST Webbook
rinpol	1617.00		NIST Webbook
ripol	2501.00		NIST Webbook
tb	643.96	K	Joback Method
tc	877.91	K	Joback Method
tf	382.94	K	Joback Method
vc	0.620	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	481.19	J/mol×K	643.96	Joback Method
cpg	501.67	J/mol×K	682.95	Joback Method
cpg	520.80	J/mol×K	721.94	Joback Method
cpg	538.58	J/mol×K	760.93	Joback Method
cpg	555.02	J/mol×K	799.93	Joback Method
cpg	570.12	J/mol×K	838.92	Joback Method
cpg	583.88	J/mol×K	877.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R136031&Units=SI
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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume