

exo-Tricyclo[6,2,1,0(2,6)]decan-8-«alpha»-ol, acetate

Inchi:	InChI=1S/C12H18O2/c1-7(13)14-12-6-8-5-11(12)10-4-2-3-9(8)10/h8-12H,2-6H2,1H3/t8?
InchiKey:	YKFHIJHJBUDXFP-MNALBRSASA-N
Formula:	C12H18O2
SMILES:	CC(=O)OC1CC2CC1C1CCCC21
Mol. weight [g/mol]:	194.27

Physical Properties

Property code	Value	Unit	Source
gf	-29.03	kJ/mol	Joback Method
hf	-364.25	kJ/mol	Joback Method
hfus	24.07	kJ/mol	Joback Method
hvap	50.75	kJ/mol	Joback Method
log10ws	-2.54		Crippen Method
logp	2.374		Crippen Method
mcvol	154.800	ml/mol	McGowan Method
pc	2563.69	kPa	Joback Method
rinpol	1414.00		NIST Webbook
rinpol	1414.00		NIST Webbook
ripol	1851.00		NIST Webbook
tb	565.40	K	Joback Method
tc	779.60	K	Joback Method
tf	338.98	K	Joback Method
vc	0.593	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	426.54	J/molxK	565.40	Joback Method
cpg	446.47	J/molxK	601.10	Joback Method
cpg	465.13	J/molxK	636.80	Joback Method
cpg	482.59	J/molxK	672.50	Joback Method
cpg	498.93	J/molxK	708.20	Joback Method
cpg	514.23	J/molxK	743.90	Joback Method
cpg	528.57	J/molxK	779.60	Joback Method

dvisc	0.0020614	Paxs	338.98	Joback Method
dvisc	0.0020742	Paxs	376.72	Joback Method
dvisc	0.0020847	Paxs	414.45	Joback Method
dvisc	0.0020935	Paxs	452.19	Joback Method
dvisc	0.0021009	Paxs	489.93	Joback Method
dvisc	0.0021074	Paxs	527.66	Joback Method
dvisc	0.0021129	Paxs	565.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R386380&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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