

exo-Tricyclo[6,2,1,0(2,6)]decan-8-«beta»-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-MUVKAJBYS-A-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	1424.00		NIST Webbook
rinpol	1424.00		NIST Webbook
ripol	1863.00		NIST Webbook
ripol	1863.00		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/mol×K	565.40	Joback Method
cpg	446.47	J/mol×K	601.10	Joback Method
cpg	465.13	J/mol×K	636.80	Joback Method
cpg	482.59	J/mol×K	672.50	Joback Method
cpg	498.93	J/mol×K	708.20	Joback Method
cpg	514.23	J/mol×K	743.90	Joback Method

cpg	528.57	J/mol×K	779.60	Joback Method
dvisc	0.0020614	Pa×s	338.98	Joback Method
dvisc	0.0020742	Pa×s	376.72	Joback Method
dvisc	0.0020847	Pa×s	414.45	Joback Method
dvisc	0.0020935	Pa×s	452.19	Joback Method
dvisc	0.0021009	Pa×s	489.93	Joback Method
dvisc	0.0021074	Pa×s	527.66	Joback Method
dvisc	0.0021129	Pa×s	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=R386404&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

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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