

Birkenal

Inchi:	InChI=1S/C14H22O/c1-10-7-14(4,9-15)6-5-12-11(10)8-13(12,2)3/h9,11-12H,1,5-8H2,2-4
InchiKey:	KHGAHZYLXXABTK-SGMGOOAPSA-N
Formula:	C14H22O
SMILES:	<chem>C=C1CC(C)(C=O)CCC2C1CC2(C)C</chem>
Mol. weight [g/mol]:	206.32

Physical Properties

Property code	Value	Unit	Source
gf	79.36	kJ/mol	Joback Method
hf	-216.71	kJ/mol	Joback Method
hfus	12.66	kJ/mol	Joback Method
hvap	51.06	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	3.594		Crippen Method
mcvol	183.670	ml/mol	McGowan Method
pc	2246.13	kPa	Joback Method
ripol	1823.00		NIST Webbook
ripol	1823.00		NIST Webbook
ripol	1823.00		NIST Webbook
tb	584.97	K	Joback Method
tc	807.47	K	Joback Method
tf	367.86	K	Joback Method
vc	0.705	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	493.28	J/molxK	584.97	Joback Method
cpg	513.79	J/molxK	622.05	Joback Method
cpg	533.06	J/molxK	659.14	Joback Method
cpg	551.32	J/molxK	696.22	Joback Method
cpg	568.81	J/molxK	733.30	Joback Method
cpg	585.77	J/molxK	770.38	Joback Method
cpg	602.43	J/molxK	807.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R340611&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
hvpap:	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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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