

Birkenol

Inchi: InChI=1S/C14H24O/c1-10-7-14(4,9-15)6-5-12-11(10)8-13(12,2)3/h11-12,15H,1,5-9H2,2-
InchiKey: YLDRPYZNHCKPGS-SGMGOOAPSA-N
Formula: C14H24O
SMILES: C=C1CC(C)(CO)CCC2C1CC2(C)C
Mol. weight [g/mol]: 208.34

Physical Properties

Property code	Value	Unit	Source
gf	42.06	kJ/mol	Joback Method
hf	-283.36	kJ/mol	Joback Method
hfus	14.46	kJ/mol	Joback Method
hvap	61.02	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	3.387		Crippen Method
mcvol	187.970	ml/mol	McGowan Method
pc	2284.95	kPa	Joback Method
ripol	2149.00		NIST Webbook
ripol	2149.00		NIST Webbook
ripol	2149.00		NIST Webbook
tb	628.49	K	Joback Method
tc	832.54	K	Joback Method
tf	386.68	K	Joback Method
vc	0.707	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	536.69	J/molxK	628.49	Joback Method
cpg	555.11	J/molxK	662.50	Joback Method
cpg	572.67	J/molxK	696.51	Joback Method
cpg	589.56	J/molxK	730.52	Joback Method
cpg	605.96	J/molxK	764.52	Joback Method
cpg	622.05	J/molxK	798.53	Joback Method
cpg	638.02	J/molxK	832.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R340626&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
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
hvp:	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
ripl:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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