Dictamnol

Inchi: InChI=1S/C12H18O/c1-9-5-3-4-6-11-10(9)7-8-12(11,2)13/h4,6,10-11,13H,1,3,5,7-8H2,2H
InchiKey: FIZZAWTVIDYQPI-HTAVTVPLSA-N
Formula: C12H18O
SMILES: C=C1CCC=CC2C1CCC2(C)O
Mol. weight [g/mol]: 178.27
CAS: 180682-30-8

Physical Properties

Property code	Value	Unit	Source
gf	56.28	kJ/mol	Joback Method
hf	-185.36	kJ/mol	Joback Method
hfus	13.63	kJ/mol	Joback Method
hvap	58.49	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	2.670		Crippen Method
mcvol	155.490	ml/mol	McGowan Method
pc	2918.68	kPa	Joback Method
ripol	2170.00		NIST Webbook
ripol	2170.00		NIST Webbook
ripol	2170.00		NIST Webbook
tb	590.59	K	Joback Method
tc	802.08	K	Joback Method
tf	341.72	K	Joback Method
vc	0.576	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	414.97	J/mol×K	590.59	Joback Method
cpg	432.06	J/mol×K	625.84	Joback Method
cpg	448.13	J/mol×K	661.09	Joback Method
cpg	463.30	J/mol×K	696.34	Joback Method
cpg	477.68	J/mol×K	731.59	Joback Method
cpg	491.41	J/mol×K	766.83	Joback Method

cpg	504.60	J/mol×K	802.08	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C180682308&Units=SI

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