«beta»-Agarofuran

Inchi: InChI=1S/C14H22O/c1-12(2)11-6-9-13(3)7-4-5-8-14(13,10-11)15-12/h5,8,11H,4,6-7,9-10
InchiKey: IEZDOTGOEOFYHV-UFPXDFCQSA-N
Formula: C14H22O
SMILES: CC1(C)OC23C=CCCC2(C)CCC1C3
Mol. weight [g/mol]: 206.32

Physical Properties

Property code	Value	Unit	Source
gf	132.61	kJ/mol	Joback Method
hf	-181.21	kJ/mol	Joback Method
hfus	11.50	kJ/mol	Joback Method
hvap	48.05	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	3.690		Crippen Method
mcvol	177.110	ml/mol	McGowan Method
pc	2581.96	kPa	Joback Method
rinpol	1516.00		NIST Webbook
rinpol	1474.00		NIST Webbook
tb	574.91	K	Joback Method
tc	819.25	K	Joback Method
tf	385.59	K	Joback Method
vc	0.666	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.55	J/mol×K	574.91	Joback Method
cpg	507.82	J/mol×K	615.63	Joback Method
cpg	528.39	J/mol×K	656.36	Joback Method
cpg	547.76	J/mol×K	697.08	Joback Method
cpg	566.42	J/mol×K	737.80	Joback Method
cpg	584.86	J/mol×K	778.53	Joback Method
cpg	603.59	J/mol×K	819.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R73054&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
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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume