furano-4(15)-eudesmen-1-one

Inchi: InChI=1S/C15H20O2/c1-9-4-5-14(16)15(3)7-13-11(6-12(9)15)10(2)8-17-13/h8,11-13H,1,
InchiKey: VWLFWHISRMKWNE-WOFVOEOOSA-N
Formula: C15H20O2
SMILES: C=C1CCC(=O)C2(C)CC3OC=C(C)C3CC12
Mol. weight [g/mol]: 232.32

Physical Properties

Property code	Value	Unit	Source
gf	60.77	kJ/mol	Joback Method
hf	-303.42	kJ/mol	Joback Method
hfus	22.55	kJ/mol	Joback Method
hvap	57.82	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.241		Crippen Method
mcvol	188.470	ml/mol	McGowan Method
pc	2289.32	kPa	Joback Method
ripol	2649.00		NIST Webbook
ripol	2649.00		NIST Webbook
tb	673.54	K	Joback Method
tc	917.23	K	Joback Method
tf	439.96	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	559.36	J/mol×K	673.54	Joback Method
cpg	580.55	J/mol×K	714.15	Joback Method
cpg	600.53	J/mol×K	754.77	Joback Method
cpg	619.50	J/mol×K	795.38	Joback Method
cpg	637.63	J/mol×K	836.00	Joback Method
cpg	655.09	J/mol×K	876.61	Joback Method
cpg	672.07	J/mol×K	917.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R395438&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume