Cedren-15-oic acid

Inchi: InChI=1S/C15H22O2/c1-9-4-5-12-14(2,3)11-8-15(9,12)7-6-10(11)13(16)17/h6,9,11-12H,
InchiKey: HRHPQHYUDVOYPI-NCLPGTSESA-N
Formula: C15H22O2
SMILES: CC1CCC2C(C)(C)C3CC12CC=C3C(=O)O
Mol. weight [g/mol]: 234.33

Physical Properties

Property code	Value	Unit	Source
gf	-38.34	kJ/mol	Joback Method
hf	-375.55	kJ/mol	Joback Method
hfus	20.88	kJ/mol	Joback Method
hvap	70.53	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	3.480		Crippen Method
mcvol	192.770	ml/mol	McGowan Method
pc	2455.60	kPa	Joback Method
rinpol	1907.00		NIST Webbook
tb	712.69	K	Joback Method
tc	927.81	K	Joback Method
tf	468.94	K	Joback Method
vc	0.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.34	J/mol×K	712.69	Joback Method
cpg	613.66	J/mol×K	748.54	Joback Method
cpg	630.54	J/mol×K	784.40	Joback Method
cpg	647.24	J/mol×K	820.25	Joback Method
cpg	664.02	J/mol×K	856.10	Joback Method
cpg	681.13	J/mol×K	891.96	Joback Method
cpg	698.83	J/mol×K	927.81	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=R516224&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume