cis-Eudesm-6-en-12-al

Inchi: InChI=1S/C15H24O/c1-11-5-4-7-15(3)8-6-13(9-14(11)15)12(2)10-16/h9-12,14H,4-8H2,1-
InchiKey: QSZPERKSHGCGQS-TYVCDUJCSA-N
Formula: C15H24O
SMILES: CC(C=O)C1=CC2C(C)CCCC2(C)CC1
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	53.69	kJ/mol	Joback Method
hf	-281.62	kJ/mol	Joback Method
hfus	16.85	kJ/mol	Joback Method
hvap	55.32	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.984		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2098.42	kPa	Joback Method
rinpol	1584.00		NIST Webbook
tb	621.09	K	Joback Method
tc	844.22	K	Joback Method
tf	340.55	K	Joback Method
vc	0.751	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	550.34	J/mol×K	621.09	Joback Method
cpg	572.08	J/mol×K	658.28	Joback Method
cpg	592.53	J/mol×K	695.47	Joback Method
cpg	611.83	J/mol×K	732.66	Joback Method
cpg	630.15	J/mol×K	769.84	Joback Method
cpg	647.63	J/mol×K	807.03	Joback Method
cpg	664.43	J/mol×K	844.22	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R198900&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

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