6,11-oxido-Acor-4-ene

Inchi: InChI=1S/C15H24O/c1-10-7-8-15-11(2)5-6-12(15)14(3,4)16-13(15)9-10/h9,11-13H,5-8H2
InchiKey: JGKMDLIITSKWAD-SFDCQRBFSA-N
Formula: C15H24O
SMILES: CC1=CC2OC(C)(C)C3CCC(C)C23CC1
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	129.18	kJ/mol	Joback Method
hf	-248.90	kJ/mol	Joback Method
hfus	21.07	kJ/mol	Joback Method
hvap	51.78	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.936		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2149.31	kPa	Joback Method
rinpol	1527.00		NIST Webbook
rinpol	1525.00		NIST Webbook
rinpol	1525.00		NIST Webbook
rinpol	1525.00		NIST Webbook
rinpol	1530.00		NIST Webbook
rinpol	1511.00		NIST Webbook
rinpol	1533.00		NIST Webbook
ripol	1830.00		NIST Webbook
tb	597.86	K	Joback Method
tc	828.69	K	Joback Method
tf	381.24	K	Joback Method
vc	0.724	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	540.74	J/mol×K	597.86	Joback Method
cpg	563.58	J/mol×K	636.33	Joback Method

cpg	584.99	J/mol×K	674.80	Joback Method
cpg	605.27	J/mol×K	713.28	Joback Method
cpg	624.73	J/mol×K	751.75	Joback Method
cpg	643.66	J/mol×K	790.22	Joback Method
cpg	662.37	J/mol×K	828.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R199889&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume