10«alpha»-Hydroxycalamenene

Inchi: InChI=1S/C15H22O/c1-10(2)12-7-8-15(4,16)14-6-5-11(3)9-13(12)14/h5-6,9-10,12,16H,7-
InchiKey: MTOMOICLIZNIAM-WPZCJLIBSA-N
Formula: C15H22O
SMILES: Cc1ccc2c(c1)C(C(C)C)CCC2(C)O
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	64.76	kJ/mol	Joback Method
hf	-235.31	kJ/mol	Joback Method
hfus	19.24	kJ/mol	Joback Method
hvap	67.50	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	3.736		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
pc	2289.32	kPa	Joback Method
rinpol	1657.00		NIST Webbook
tb	677.56	K	Joback Method
tc	887.88	K	Joback Method
tf	390.17	K	Joback Method
vc	0.727	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	546.94	J/mol×K	677.56	Joback Method
cpg	563.77	J/mol×K	712.61	Joback Method
cpg	579.80	J/mol×K	747.67	Joback Method
cpg	595.17	J/mol×K	782.72	Joback Method
cpg	610.00	J/mol×K	817.77	Joback Method
cpg	624.42	J/mol×K	852.83	Joback Method
cpg	638.55	J/mol×K	887.88	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=R233751&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