«alpha»-Acorenol

Other names: Acorenol
Inchi: InChI=1S/C15H26O/c1-11-7-9-15(10-8-11)12(2)5-6-13(15)14(3,4)16/h7,12-13,16H,5-6,8-
InchiKey: XDVDHFJMCJWDPI-RLSDIYDTSA-N
Formula: C15H26O
SMILES: CC1=CCC2(CC1)C(C)CCC2C(C)(C)O
Mol. weight [g/mol]: 222.37
CAS: 28296-85-7

Physical Properties

Property code	Value	Unit	Source
gf	21.67	kJ/mol	Joback Method
hf	-351.74	kJ/mol	Joback Method
hfus	14.76	kJ/mol	Joback Method
hvap	64.38	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	3.920		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
pc	2155.30	kPa	Joback Method
rinpol	1616.00		NIST Webbook
rinpol	1630.00		NIST Webbook
rinpol	1616.00		NIST Webbook
rinpol	1633.00		NIST Webbook
rinpol	1629.00		NIST Webbook
rinpol	1634.00		NIST Webbook
rinpol	1630.00		NIST Webbook
rinpol	1630.00		NIST Webbook
rinpol	1630.00		NIST Webbook
rinpol	1632.00		NIST Webbook
rinpol	1626.00		NIST Webbook
rinpol	1621.00		NIST Webbook
rinpol	1605.00		NIST Webbook
rinpol	1631.00		NIST Webbook
rinpol	1630.00		NIST Webbook
rinpol	1633.00		NIST Webbook
rinpol	1630.00		NIST Webbook
rinpol	1612.00		NIST Webbook
rinpol	1626.00		NIST Webbook

rinpol	1628.00		NIST Webbook
rinpol	1630.00		NIST Webbook
rinpol	1630.00		NIST Webbook
rinpol	1614.00		NIST Webbook
rinpol	1630.00		NIST Webbook
rinpol	1627.00		NIST Webbook
rinpol	1630.00		NIST Webbook
rinpol	1633.00		NIST Webbook
ripol	2127.00		NIST Webbook
ripol	2123.00		NIST Webbook
ripol	2163.00		NIST Webbook
ripol	2163.00		NIST Webbook
ripol	2124.00		NIST Webbook
ripol	2163.00		NIST Webbook
tb	661.82	K	Joback Method
tc	874.07	K	Joback Method
tf	376.79	K	Joback Method
vc	0.749	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.13	J/mol×K	661.82	Joback Method
cpg	618.08	J/mol×K	697.19	Joback Method
cpg	636.92	J/mol×K	732.57	Joback Method
cpg	654.81	J/mol×K	767.94	Joback Method
cpg	671.91	J/mol×K	803.32	Joback Method
cpg	688.38	J/mol×K	838.69	Joback Method
cpg	704.35	J/mol×K	874.07	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C28296857&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