

«beta»-Atlantol

Inchi: InChI=1S/C15H24O/c1-11(2)9-15(16)10-13(4)14-7-5-12(3)6-8-14/h5,9,14-16H,4,6-8,10H
InchiKey: HGURSBWDVNEOKP-UHFFFAOYSA-N
Formula: C15H24O
SMILES: C=C(CC(O)C=C(C)C)C1CC=C(C)CC1
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
hfus	24.14	kJ/mol	Joback Method
hvap	81.21	kJ/mol	Cheméo Relay (1.0)
ie	8.46	eV	Cheméo Relay (1.0)
log10ws	-3.41		Cheméo Relay (1.0)
logp	4.006		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
rinpol	1608.00		NIST Webbook
rinpol	1608.00		NIST Webbook
rinpol	1608.00		NIST Webbook
tb	569.98	K	Cheméo Relay (1.0)
tf	322.45	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	564.15	J/mol×K	658.63	Joback Method
cpg	581.55	J/mol×K	691.59	Joback Method
cpg	597.98	J/mol×K	724.55	Joback Method
cpg	613.46	J/mol×K	757.52	Joback Method
cpg	628.07	J/mol×K	790.48	Joback Method
cpg	641.84	J/mol×K	823.44	Joback Method
cpg	654.82	J/mol×K	856.40	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R401895&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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