

Ambroxide

Other names:	8 «alpha»,12-epoxy-13,14,15,16-tertanorlabdane [3aR-(3a«alpha»,5a«beta»,9a«alpha»,9b«beta»)]-dodecahydro-3a,6,6,9a-tetramethylna
Inchi:	InChI=1S/C16H28O/c1-14(2)8-5-9-15(3)12(14)6-10-16(4)13(15)7-11-17-16/h12-13H,5-1
InchiKey:	YPZUZOLGGMJZJO-ZMLGBVNGSA-N
Formula:	C16H28O
SMILES:	CC1(C)CCCC2(C)C1CCC1(C)OCCC12
Mol. weight [g/mol]:	236.39
CAS:	6790-58-5

Physical Properties

Property code	Value	Unit	Source
gf	99.68	kJ/mol	Joback Method
hf	-306.77	kJ/mol	Joback Method
hfus	14.43	kJ/mol	Joback Method
hvap	52.08	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	4.408		Crippen Method
mcvol	209.590	ml/mol	McGowan Method
pc	2058.62	kPa	Joback Method
rinpwl	1749.00		NIST Webbook
rinpwl	1749.00		NIST Webbook
ripwl	2200.00		NIST Webbook
tb	621.11	K	Joback Method
tc	861.29	K	Joback Method
tf	399.61	K	Joback Method
vc	0.783	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	615.45	J/molxK	621.11	Joback Method
cpg	640.98	J/molxK	661.14	Joback Method
cpg	665.10	J/molxK	701.17	Joback Method
cpg	688.26	J/molxK	741.20	Joback Method

cpg	710.91	J/mol×K	781.23	Joback Method
cpg	733.52	J/mol×K	821.26	Joback Method
cpg	756.55	J/mol×K	861.29	Joback Method

Sources

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=C6790585&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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