Ambrox

Inchi: InChI=1S/C15H26O/c1-14(2)8-4-9-15(3)11-7-10-16-12(11)5-6-13(14)15/h11-13H,4-10H2
InchiKey: IPEPBOBQYDJNON-UHFFFAOYSA-N
Formula: C15H26O
SMILES: CC1(C)CCCC2(C)C3CCOC3CCC12
Mol. weight [g/mol]: 222.37
CAS: 65588-69-4

Physical Properties

Property code	Value	Unit	Source
gf	96.75	kJ/mol	Joback Method
hf	-301.37	kJ/mol	Joback Method
hfus	18.14	kJ/mol	Joback Method
hvap	51.00	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	4.018		Crippen Method
mcvol	195.500	ml/mol	McGowan Method
pc	2157.31	kPa	Joback Method
rinpol	1748.00		NIST Webbook
rinpol	1756.00		NIST Webbook
ripol	2199.00		NIST Webbook
tb	597.99	K	Joback Method
tc	833.63	K	Joback Method
tf	364.44	K	Joback Method
vc	0.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	563.04	J/mol×K	597.99	Joback Method
cpg	588.46	J/mol×K	637.26	Joback Method
cpg	612.24	J/mol×K	676.54	Joback Method
cpg	634.70	J/mol×K	715.81	Joback Method
cpg	656.16	J/mol×K	755.09	Joback Method
cpg	676.92	J/mol×K	794.36	Joback Method

cpg	697.32	J/mol×K	833.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C65588694&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

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