

(E)-amylcinnamic alcohol

Inchi:	InChI=1S/C14H20O/c1-2-3-5-10-14(12-15)11-13-8-6-4-7-9-13/h4,6-9,11,15H,2-3,5,10,12
InchiKey:	LIPHCKNQPJXUQF-SDNWHVSQSA-N
Formula:	C14H20O
SMILES:	CCCCC(=Cc1cccc1)CO
Mol. weight [g/mol]:	204.31

Physical Properties

Property code	Value	Unit	Source
gf	114.26	kJ/mol	Joback Method
hf	-140.56	kJ/mol	Joback Method
hfus	29.04	kJ/mol	Joback Method
hvap	65.75	kJ/mol	Joback Method
log10ws	-4.07		Crippen Method
logp	3.643		Crippen Method
mcvol	185.930	ml/mol	McGowan Method
pc	2306.95	kPa	Joback Method
rinpol	1617.00		NIST Webbook
rinpol	1617.00		NIST Webbook
tb	642.62	K	Joback Method
tc	836.25	K	Joback Method
tf	315.74	K	Joback Method
vc	0.712	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	486.74	J/mol×K	642.62	Joback Method
cpg	501.41	J/mol×K	674.89	Joback Method
cpg	515.24	J/mol×K	707.16	Joback Method
cpg	528.29	J/mol×K	739.44	Joback Method
cpg	540.61	J/mol×K	771.71	Joback Method
cpg	552.24	J/mol×K	803.98	Joback Method
cpg	563.23	J/mol×K	836.25	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=R513681&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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