

cinnamyl benzoate

Inchi:	InChI=1S/C16H14O2/c17-16(15-11-5-2-6-12-15)18-13-7-10-14-8-3-1-4-9-14/h1-12H,13H
InchiKey:	UARVBDPGNUHYQT-JXMROGBWSA-N
Formula:	C16H14O2
SMILES:	O=C(OCC=Cc1ccccc1)c1ccccc1
Mol. weight [g/mol]:	238.28
CAS:	5320-75-2

Physical Properties

Property code	Value	Unit	Source
gf	154.96	kJ/mol	Joback Method
hf	-28.09	kJ/mol	Joback Method
hfus	28.27	kJ/mol	Joback Method
hvap	64.88	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	3.557		Crippen Method
mcvol	191.920	ml/mol	McGowan Method
pc	2515.07	kPa	Joback Method
rinpol	2024.00		NIST Webbook
rinpol	2024.00		NIST Webbook
rinpol	2033.00		NIST Webbook
tb	699.29	K	Joback Method
tc	941.67	K	Joback Method
tf	390.00	K	Joback Method
vc	0.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	495.69	J/mol×K	699.29	Joback Method
cpg	561.58	J/mol×K	901.28	Joback Method
cpg	550.60	J/mol×K	860.88	Joback Method
cpg	538.61	J/mol×K	820.48	Joback Method
cpg	525.51	J/mol×K	780.08	Joback Method
cpg	511.23	J/mol×K	739.69	Joback Method

cpg	571.63	J/mol×K	941.67	Joback Method
dvisc	0.0001055	Pa×s	699.29	Joback Method
dvisc	0.0001359	Pa×s	647.74	Joback Method
dvisc	0.0001830	Pa×s	596.19	Joback Method
dvisc	0.0002607	Pa×s	544.64	Joback Method
dvisc	0.0003999	Pa×s	493.10	Joback Method
dvisc	0.0006777	Pa×s	441.55	Joback Method
dvisc	0.0013204	Pa×s	390.00	Joback Method

Sources

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=C5320752&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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