

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	2033.00		NIST Webbook
rinpol	2024.00		NIST Webbook
rinpol	2024.00		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/molxK	699.29	Joback Method
cpg	511.23	J/molxK	739.69	Joback Method
cpg	525.51	J/molxK	780.08	Joback Method
cpg	538.61	J/molxK	820.48	Joback Method
cpg	550.60	J/molxK	860.88	Joback Method
cpg	561.58	J/molxK	901.28	Joback Method

cpg	571.63	J/molxK	941.67	Joback Method
dvisc	0.0013204	Paxs	390.00	Joback Method
dvisc	0.0006777	Paxs	441.55	Joback Method
dvisc	0.0003999	Paxs	493.10	Joback Method
dvisc	0.0002607	Paxs	544.64	Joback Method
dvisc	0.0001830	Paxs	596.19	Joback Method
dvisc	0.0001359	Paxs	647.74	Joback Method
dvisc	0.0001055	Paxs	699.29	Joback Method

Sources

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/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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