

C16H18

Inchi:	InChI=1S/C16H18/c1-14(16-10-6-3-7-11-16)12-13-15-8-4-2-5-9-15/h2-11,14H,12-13H2,1
InchiKey:	PDINXYLAVFUHSA-CQSZACIVSA-N
Formula:	C16H18
SMILES:	CC(CCc1ccccc1)c1ccccc1
Mol. weight [g/mol]:	210.31
CAS:	17293-55-9

Physical Properties

Property code	Value	Unit	Source
gf	306.22	kJ/mol	Joback Method
hf	94.21	kJ/mol	Joback Method
hfus	21.76	kJ/mol	Joback Method
hvap	55.37	kJ/mol	Joback Method
log10ws	-4.69		Crippen Method
logp	4.423		Crippen Method
mcvol	188.780	ml/mol	McGowan Method
pc	2302.53	kPa	Joback Method
tb	618.40	K	Joback Method
tc	853.40	K	Joback Method
tf	307.92	K	Joback Method
vc	0.710	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.73	J/molxK	618.40	Joback Method
cpg	491.86	J/molxK	657.57	Joback Method
cpg	509.59	J/molxK	696.73	Joback Method
cpg	525.99	J/molxK	735.90	Joback Method
cpg	541.15	J/molxK	775.06	Joback Method
cpg	555.14	J/molxK	814.23	Joback Method
cpg	568.06	J/molxK	853.40	Joback Method
dvisc	0.0032193	Paxs	307.92	Joback Method
dvisc	0.0013116	Paxs	359.67	Joback Method

dvisc	0.0006698	Paxs	411.41	Joback Method
dvisc	0.0003975	Paxs	463.16	Joback Method
dvisc	0.0002620	Paxs	514.91	Joback Method
dvisc	0.0001863	Paxs	566.65	Joback Method
dvisc	0.0001403	Paxs	618.40	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=C17293559&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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