

ETHYL DIPHENYLCARBAMATE

Other names:	N,N-Diphenylurethane N,N-Diphenylethyl carbamate Carbamic acid, diphenyl-, ethyl ester Diphenylcarbamic acid, ethyl ester Diphenylurethane Ethyl diphenylcarbamate N,N-Diphenyl carbamic acid, ethyl ester
Inchi:	InChI=1S/C15H15NO2/c1-2-18-15(17)16(13-9-5-3-6-10-13)14-11-7-4-8-12-14/h3-12H,2H
InchiKey:	HKTSLDUAGCAISP-UHFFFAOYSA-N
Formula:	C15H15NO2
SMILES:	CCOC(=O)N(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	241.29

Physical Properties

Property code	Value	Unit	Source
af	0.6451		Cheméo Relay (1.0)
chs	-7765.50 ± 7.90	kJ/mol	NIST Webbook
chs	-7785.21	kJ/mol	NIST Webbook
chs	-7740.40	kJ/mol	NIST Webbook
hf	-167.94	kJ/mol	Cheméo Relay (1.0)
hfs	-261.20	kJ/mol	NIST Webbook
hfs	-281.00 ± 7.90	kJ/mol	NIST Webbook
hfs	-290.00	kJ/mol	NIST Webbook
hfus	28.50	kJ/mol	Joback Method
hvap	83.31	kJ/mol	Cheméo Relay (1.0)
ie	8.04	eV	Cheméo Relay (1.0)
log10ws	-3.91		Cheméo Relay (1.0)
logp	3.981		Crippen Method
mcvol	192.110	ml/mol	McGowan Method
pc	2624.46	kPa	Joback Method
tb	633.20	K	NIST Webbook
tc	876.39	K	Cheméo Relay (1.0)
tf	327.38	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	505.22	J/mol×K	684.69	Joback Method
cpg	521.19	J/mol×K	723.67	Joback Method
cpg	535.88	J/mol×K	762.64	Joback Method
cpg	549.35	J/mol×K	801.62	Joback Method
cpg	561.69	J/mol×K	840.59	Joback Method
cpg	572.95	J/mol×K	879.57	Joback Method
cpg	583.21	J/mol×K	918.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C603521&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature

tc: Critical Temperature
tf: Normal melting (fusion) point

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