

2,2'-Diethyldiphenylamine

Other names:	2-ethyl-N-(2-ethylphenyl)aniline
Inchi:	InChI=1S/C16H19N/c1-3-13-9-5-7-11-15(13)17-16-12-8-6-10-14(16)4-2/h5-12,17H,3-4H2
InchiKey:	RZFNPHWOOGJMQE-UHFFFAOYSA-N
Formula:	C16H19N
SMILES:	CCc1ccccc1Nc1ccccc1CC
Mol. weight [g/mol]:	225.33
CAS:	64653-59-4

Physical Properties

Property code	Value	Unit	Source
gf	378.79	kJ/mol	Joback Method
hf	130.02	kJ/mol	Joback Method
hfus	29.60	kJ/mol	Joback Method
hvap	63.52	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	4.555		Crippen Method
mcvol	198.760	ml/mol	McGowan Method
pc	2248.26	kPa	Joback Method
rinpol	1814.30		NIST Webbook
tb	678.97	K	Joback Method
tc	908.92	K	Joback Method
tf	400.62	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	526.47	J/molxK	678.97	Joback Method
cpg	543.82	J/molxK	717.30	Joback Method
cpg	559.95	J/molxK	755.62	Joback Method
cpg	574.94	J/molxK	793.95	Joback Method
cpg	588.84	J/molxK	832.27	Joback Method
cpg	601.72	J/molxK	870.60	Joback Method
cpg	613.65	J/molxK	908.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C64653594&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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