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]: 225.34

Physical Properties

Property code	Value	Unit	Source
af	0.6149		Cheméo Relay (1.0)
gf	378.79	kJ/mol	Joback Method
hf	71.42	kJ/mol	Cheméo Relay (1.0)
hfus	29.60	kJ/mol	Joback Method
hvap	87.17	kJ/mol	Cheméo Relay (1.0)
ie	7.24	eV	Cheméo Relay (1.0)
log10ws	-4.98		Cheméo Relay (1.0)
logp	4.555		Crippen Method
mcvol	198.760	ml/mol	McGowan Method
pc	2248.26	kPa	Joback Method
rinpol	1814.30		NIST Webbook
rinpol	1814.30		NIST Webbook
tb	604.65	K	Cheméo Relay (1.0)
tc	876.34	K	Cheméo Relay (1.0)
tf	302.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)
vc	0.718	m3/kmol	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K

Coeff. A	-5.20780e+01
Coeff. B	1.32324e+00
Coeff. C	-8.23520e-04
Coeff. D	1.90900e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

Cheméo Relay (1.0, beta):

Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Datset/1031637
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C64653594&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):

Legend

af:	Acentric Factor
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
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
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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