

N-(2-ethylhexyl)aniline

Inchi:	InChI=1S/C14H23N/c1-3-5-9-13(4-2)12-15-14-10-7-6-8-11-14/h6-8,10-11,13,15H,3-5,9,1
InchiKey:	GXFHZISVUPJOCI-UHFFFAOYSA-N
Formula:	C14H23N
SMILES:	CCCCC(CC)CNc1ccccc1
Mol. weight [g/mol]:	205.35
CAS:	10137-80-1

Physical Properties

Property code	Value	Unit	Source
af	0.5848		Cheméo Relay (1.0)
hf	-71.41	kJ/mol	Cheméo Relay (1.0)
hfus	27.63	kJ/mol	Joback Method
hvap	72.68	kJ/mol	Cheméo Relay (1.0)
ie	7.28	eV	Cheméo Relay (1.0)
log10ws	-4.64		Cheméo Relay (1.0)
logp	4.315		Crippen Method
mcvol	194.340	ml/mol	McGowan Method
pc	2047.46	kPa	Joback Method
tb	566.46	K	Cheméo Relay (1.0)
tc	778.79	K	Cheméo Relay (1.0)
tf	245.82	K	Cheméo Relay (1.0)
vc	0.682	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.17	J/mol×K	596.13	Joback Method
cpg	517.27	J/mol×K	629.26	Joback Method
cpg	534.35	J/mol×K	662.39	Joback Method
cpg	550.47	J/mol×K	695.52	Joback Method
cpg	565.66	J/mol×K	728.65	Joback Method
cpg	579.97	J/mol×K	761.78	Joback Method
cpg	593.43	J/mol×K	794.91	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.38573e+01
Coeff. B	-4.31162e+03
Coeff. C	-9.23400e+01
Temperature range (K), min.	410.08
Temperature range (K), max.	596.87

Sources

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor
Pressure:
Joback Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

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
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
pvap:	Vapor pressure

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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