p-Hexadecyloxyaniline

Other names: 4-n-Hexadecyloxyaniline
p-Hexadecyloxyaniline
Inchi: InChI=1S/C22H39NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-20-24-22-18-16-21(23)17-19
InchiKey: DETPMDIIFZGDAE-UHFFFAOYSA-N
Formula: C22H39NO
SMILES: CCCCCCCCCCCCCCCCOc1ccc(N)cc1
Mol. weight [g/mol]: 333.56

Physical Properties

Property code	Value	Unit	Source
af	1.0764		Cheméo Relay (1.0)
hfus	52.77	kJ/mol	Joback Method
hvap	117.84	kJ/mol	Cheméo Relay (1.0)
ie	7.73	eV	Cheméo Relay (1.0)
log10ws	-7.23		Cheméo Relay (1.0)
logp	7.129		Crippen Method
mcvol	312.930	ml/mol	McGowan Method
pc	1130.62	kPa	Joback Method
tb	670.66	K	Cheméo Relay (1.0)
tc	859.63	K	Cheméo Relay (1.0)
tf	343.26	K	Cheméo Relay (1.0)
vc	1.189	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	998.58	J/mol×K	829.37	Joback Method
cpg	1017.72	J/mol×K	861.79	Joback Method
cpg	1035.73	J/mol×K	894.21	Joback Method
cpg	1052.67	J/mol×K	926.63	Joback Method
cpg	1068.57	J/mol×K	959.05	Joback Method
cpg	1083.47	J/mol×K	991.47	Joback Method
cpg	1097.43	J/mol×K	1023.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7502069&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
cpg:	Ideal gas heat capacity
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
vc:	Critical Volume