4-(Hexadecyloxy)aniline

Other names: p-Hexadecyloxyaniline
4-n-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]: 333.55
CAS: 7502-06-9

Physical Properties

Property code	Value	Unit	Source
gf	198.59	kJ/mol	Joback Method
hf	-370.78	kJ/mol	Joback Method
hfus	52.77	kJ/mol	Joback Method
hvap	80.55	kJ/mol	Joback Method
log10ws	-7.50		Crippen Method
logp	7.129		Crippen Method
mcvol	312.930	ml/mol	McGowan Method
pc	1130.62	kPa	Joback Method
tb	829.37	K	Joback Method
tc	1023.89	K	Joback Method
tf	482.13	K	Joback Method
vc	1.206	m3/kmol	Joback Method

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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7502069&Units=SI

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

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