p-Heptyloxyaniline

Other names: 4-n-Heptyloxyaniline
Inchi: InChI=1S/C13H21NO/c1-2-3-4-5-6-11-15-13-9-7-12(14)8-10-13/h7-10H,2-6,11,14H2,1H3
InchiKey: LTGYTOOKQWFTQG-UHFFFAOYSA-N
Formula: C13H21NO
SMILES: CCCCCCCOc1ccc(N)cc1
Mol. weight [g/mol]: 207.31
CAS: 39905-44-7

Physical Properties

Property code	Value	Unit	Source
gf	122.81	kJ/mol	Joback Method
hf	-185.02	kJ/mol	Joback Method
hfus	29.46	kJ/mol	Joback Method
hvap	60.52	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.618		Crippen Method
mcvol	186.120	ml/mol	McGowan Method
pc	2246.13	kPa	Joback Method
tb	623.45	K	Joback Method
tc	827.90	K	Joback Method
tf	380.70	K	Joback Method
vc	0.703	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	487.58	J/mol×K	623.45	Joback Method
cpg	503.93	J/mol×K	657.52	Joback Method
cpg	519.39	J/mol×K	691.60	Joback Method
cpg	533.98	J/mol×K	725.67	Joback Method
cpg	547.73	J/mol×K	759.75	Joback Method
cpg	560.67	J/mol×K	793.82	Joback Method
cpg	572.82	J/mol×K	827.90	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	419.00 ± 1.00	K	0.07	NIST Webbook

Sources

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=C39905447&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume