Aniline, n-sec-octyl-

Inchi: InChI=1S/C14H23N/c1-3-4-5-7-10-13(2)15-14-11-8-6-9-12-14/h6,8-9,11-13,15H,3-5,7,10
InchiKey: PLMXQTQKTSWGSY-UHFFFAOYSA-N
Formula: C14H23N
SMILES: CCCCCCC(C)Nc1ccccc1
Mol. weight [g/mol]: 205.34
CAS: 29675-81-8

Physical Properties

Property code	Value	Unit	Source
gf	266.36	kJ/mol	Joback Method
hf	-47.57	kJ/mol	Joback Method
hfus	27.63	kJ/mol	Joback Method
hvap	55.08	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	4.457		Crippen Method
mcvol	194.340	ml/mol	McGowan Method
pc	2047.46	kPa	Joback Method
tb	596.13	K	Joback Method
tc	794.91	K	Joback Method
tf	311.62	K	Joback Method
vc	0.741	m3/kmol	Joback Method

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

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=C29675818&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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