

3,4-Dichloro-n-dodecylaniline

Inchi:	InChI=1S/C18H29Cl2N/c1-2-3-4-5-6-7-8-9-10-11-14-21-16-12-13-17(19)18(20)15-16/h12
InchiKey:	FBLLQVUJLWZRRG-UHFFFAOYSA-N
Formula:	C18H29Cl2N
SMILES:	CCCCCCCCCCCCNc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]:	330.34
CAS:	116436-28-3

Physical Properties

Property code	Value	Unit	Source
gf	259.36	kJ/mol	Joback Method
hf	-179.27	kJ/mol	Joback Method
hfus	49.13	kJ/mol	Joback Method
hvap	74.47	kJ/mol	Joback Method
log10ws	-7.46		Crippen Method
logp	7.326		Crippen Method
mcvol	275.180	ml/mol	McGowan Method
pc	1365.67	kPa	Joback Method
tb	772.91	K	Joback Method
tc	970.38	K	Joback Method
tf	456.58	K	Joback Method
vc	1.069	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	779.84	J/molxK	772.91	Joback Method
cpg	796.50	J/molxK	805.82	Joback Method
cpg	812.20	J/molxK	838.73	Joback Method
cpg	826.99	J/molxK	871.65	Joback Method
cpg	840.91	J/molxK	904.56	Joback Method
cpg	854.01	J/molxK	937.47	Joback Method
cpg	866.33	J/molxK	970.38	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=C116436283&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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