

Tiocarlide

Other names:

Thiourea, N,N'-bis[4-(3-methylbutoxy)phenyl]-
Carbanilide, 4,4'-bis(isopentyloxy)thio-
4,4'-Diisoamyloxythiocarbanilide
Isoxyl
Thiocarlide
Tiocarlid
4,4'-Bis(isopentyloxy)thiocarbanilide
Datanil
DATC
Disocarban
4,4'-Bis(isoamyloxy)thiocarbanilide

Inchi:

InChI=1S/C23H32N2O2S/c1-17(2)13-15-26-21-9-5-19(6-10-21)24-23(28)25-20-7-11-22(

InchiKey:

BWBONKHPVHMQHE-UHFFFAOYSA-N

Formula:

C23H32N2O2S

SMILES:

CC(C)CCOc1ccc(NC(=S)Nc2ccc(OCCC(C)C)cc2)cc1

Mol. weight [g/mol]:

400.58

CAS:

910-86-1

Physical Properties

Property code	Value	Unit	Source
gf	429.30	kJ/mol	Joback Method
hf	-89.49	kJ/mol	Joback Method
hfus	52.76	kJ/mol	Joback Method
hvap	96.31	kJ/mol	Joback Method
log10ws	-7.17		Crippen Method
logp	6.345		Crippen Method
mcvol	331.160	ml/mol	McGowan Method
pc	1377.86	kPa	Joback Method
tb	1003.30	K	Joback Method
tc	1237.71	K	Joback Method
tf	580.90	K	Joback Method
vc	1.238	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1070.86	J/mol×K	1003.30	Joback Method
cpg	1085.85	J/mol×K	1042.37	Joback Method
cpg	1099.70	J/mol×K	1081.44	Joback Method
cpg	1112.52	J/mol×K	1120.50	Joback Method
cpg	1124.41	J/mol×K	1159.57	Joback Method
cpg	1135.47	J/mol×K	1198.64	Joback Method
cpg	1145.79	J/mol×K	1237.71	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C910861&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

Latest version available from:

<https://www.chemeo.com/cid/118-812-9/Tiocarlide.pdf>

Generated by Cheméo on 2024-05-03 01:50:20.716174257 +0000 UTC m=+16990269.636751573.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.