

THIOCARLIDE

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]:	400.59

Physical Properties

Property code	Value	Unit	Source
hfus	52.76	kJ/mol	Joback Method
logp	6.345		Crippen Method
mcvol	331.160	ml/mol	McGowan 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:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C910861&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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