

Orbencarb

Other names:

Carbamic acid, diethylthio-, S-(o-chlorobenzyl) ester

B 3356

Carbamothioic acid, diethyl-, S-((2-chlorophenyl)methyl) ester

S-(2-Chlorobenzyl)-N,N-diethylthiolcarbamate

Diethylthiocarbamic acid S-(o-chlorobenzyl) ester

Lanray

Orthobencarb

Carbamothioic acid, N,N-diethyl-, S-[(2-chlorophenyl)methyl] ester

Inchi: InChI=1S/C12H16ClNOS/c1-3-14(4-2)12(15)16-9-10-7-5-6-8-11(10)13/h5-8H,3-4,9H2,1-**InchiKey:** LLLFASISUZUJEQ-UHFFFAOYSA-N**Formula:** C12H16ClNOS**SMILES:** CCN(CC)C(=O)SCc1ccccc1Cl**Mol. weight [g/mol]:** 257.78**CAS:** 34622-58-7

Physical Properties

Property code	Value	Unit	Source
gf	155.99	kJ/mol	Joback Method
hf	-84.87	kJ/mol	Joback Method
hfus	33.43	kJ/mol	Joback Method
hvap	65.23	kJ/mol	Joback Method
log10ws	-4.34		Crippen Method
logp	4.035		Crippen Method
mcvol	196.320	ml/mol	McGowan Method
pc	2467.81	kPa	Joback Method
tb	678.14	K	Joback Method
tc	904.46	K	Joback Method
tf	410.66	K	Joback Method
vc	0.727	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	486.62	J/molxK	678.14	Joback Method

cpg	500.93	J/mol×K	715.86	Joback Method
cpg	514.20	J/mol×K	753.58	Joback Method
cpg	526.49	J/mol×K	791.30	Joback Method
cpg	537.84	J/mol×K	829.02	Joback Method
cpg	548.30	J/mol×K	866.74	Joback Method
cpg	557.91	J/mol×K	904.46	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=C34622587&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
h vap:	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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