

Clobenzorex

Other names:	Asenlix Finedal Benzeneethanamine, N-[(2-chlorophenyl)methyl]-«alpha»-methyl-, (+)- Dinintel (+)-N-(o-Chlorobenzyl)-«alpha»-methylphenethylamine SD 271-12 N-(2-Chlorobenzyl)-1-phenyl-2-propanamine-, (+)- Benzenemethanamine, 2'-chloro, N-(1-methyl-2-phenylethyl), (+)- 5843-53-8 (hydrochloride) Benzenemethanamine, 2'-chloro, N-(1-methyl-2-phenylethyl)
Inchi:	InChI=1S/C16H18ClN/c1-13(11-14-7-3-2-4-8-14)18-12-15-9-5-6-10-16(15)17/h2-10,13,15,16,17,18
InchiKey:	LRXXRIXDSAEIOR-UHFFFAOYSA-N
Formula:	C16H18ClN
SMILES:	CC(Cc1ccccc1)NCc1ccccc1Cl
Mol. weight [g/mol]:	259.77
CAS:	13364-32-4

Physical Properties

Property code	Value	Unit	Source
gf	374.05	kJ/mol	Joback Method
hf	120.47	kJ/mol	Joback Method
hfus	30.66	kJ/mol	Joback Method
hvap	66.86	kJ/mol	Joback Method
log10ws	-5.21		Crippen Method
logp	4.061		Crippen Method
mcvol	211.000	ml/mol	McGowan Method
pc	2218.71	kPa	Joback Method
tb	710.98	K	Joback Method
tc	947.34	K	Joback Method
tf	403.02	K	Joback Method
vc	0.793	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	555.46	J/mol×K	710.98	Joback Method
cpg	571.96	J/mol×K	750.37	Joback Method
cpg	587.19	J/mol×K	789.77	Joback Method
cpg	601.23	J/mol×K	829.16	Joback Method
cpg	614.17	J/mol×K	868.55	Joback Method
cpg	626.08	J/mol×K	907.95	Joback Method
cpg	637.05	J/mol×K	947.34	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C13364324&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
mccvol:	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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