

Thozalinone

Other names:	2-(Dimethylamino)-5-phenyl-2-oxazolin-4-one CL 39808 Stimsen Tozalinone 2-Oxazolin-4-one, 2-(dimethylamino)-5-phenyl-4(5H)-Oxazolone, 2-(dimethylamino)-5-phenyl-5-Phenyl-2-(dimethylamino)-2-oxazolin-4-one Dimethyl derivative of Pemoline 2-(Dimethylamino)-5-phenyl-1,3-oxazol-4(5H)-one NSC 170962
Inchi:	InChI=1S/C11H12N2O2/c1-13(2)11-12-10(14)9(15-11)8-6-4-3-5-7-8/h3-7,9H,1-2H3
InchiKey:	JJSHYECKYLDYAR-UHFFFAOYSA-N
Formula:	C11H12N2O2
SMILES:	CN(C)C1=NC(=O)C(c2ccccc2)O1
Mol. weight [g/mol]:	204.23
CAS:	655-05-0

Physical Properties

Property code	Value	Unit	Source
gf	229.88	kJ/mol	Joback Method
hf	-58.25	kJ/mol	Joback Method
hfus	28.70	kJ/mol	Joback Method
hvap	60.58	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	1.202		Crippen Method
mcvol	154.330	ml/mol	McGowan Method
pc	3392.03	kPa	Joback Method
rinpol	2040.00		NIST Webbook
rinpol	2040.00		NIST Webbook
tb	658.09	K	Joback Method
tc	912.26	K	Joback Method
tf	463.13	K	Joback Method
vc	0.566	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	428.22	J/molxK	658.09	Joback Method
cpg	445.58	J/molxK	700.45	Joback Method
cpg	461.54	J/molxK	742.81	Joback Method
cpg	476.09	J/molxK	785.17	Joback Method
cpg	489.25	J/molxK	827.53	Joback Method
cpg	501.02	J/molxK	869.90	Joback Method
cpg	511.41	J/molxK	912.26	Joback Method

Sources

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=C655050&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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