

Metaxalone

Other names:	2-Oxazolidinone, 5-((3,5-xylyloxy)methyl)- 2-Oxazolidinone, 5-[(3,5-dimethylphenoxy)methyl]- 5-((3,5-Dimethylphenoxy)methyl)-2-oxazolidinone 5-((3,5-Xylyloxy)methyl)-2-oxazolidinone 5-((3,5-dimethylphenoxy)methyl)oxazolidin-2-one 5-(3,5-Xyloloxymethyl)oxazolidin-2-one 5-[(3,5-dimethylphenoxy)methyl]-2-oxazolidinone AHR-438 CL 39,148 Metaxalon Metaxolone Metazalone Metazolone Methaxalonum Methoxolone NSC 170959 Skelaxin Zorane
Inchi:	InChI=1S/C12H15NO3/c1-8-3-9(2)5-10(4-8)15-7-11-6-13-12(14)16-11/h3-5,11H,6-7H2,1
InchiKey:	IMWZZHHPURKASS-UHFFFAOYSA-N
Formula:	C12H15NO3
SMILES:	Cc1cc(C)cc(OCC2CN=C(O)O2)c1
Mol. weight [g/mol]:	221.25
CAS:	1665-48-1

Physical Properties

Property code	Value	Unit	Source
gf	-10.97	kJ/mol	Joback Method
hf	-316.11	kJ/mol	Joback Method
hfus	33.26	kJ/mol	Joback Method
hvap	76.93	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	1.995		Crippen Method
mcvol	168.610	ml/mol	McGowan Method
pc	3082.99	kPa	Joback Method
rinpol	2163.00		NIST Webbook
rinpol	2221.80		NIST Webbook

rinpol	2163.00		NIST Webbook
rinpol	2145.00		NIST Webbook
rinpol	2221.80		NIST Webbook
tb	725.27	K	Joback Method
tc	945.06	K	Joback Method
tf	481.80	K	Joback Method
vc	0.633	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	493.87	J/mol×K	725.27	Joback Method
cpg	507.84	J/mol×K	761.90	Joback Method
cpg	520.80	J/mol×K	798.53	Joback Method
cpg	532.75	J/mol×K	835.16	Joback Method
cpg	543.69	J/mol×K	871.80	Joback Method
cpg	553.63	J/mol×K	908.43	Joback Method
cpg	562.57	J/mol×K	945.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1665481&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility correlation and thermodynamic analysis of two forms of water in different pure solvents:	https://www.doi.org/10.1016/j.fluid.2015.09.013
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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