Mesurol sulfoxide

Other names:	Phenol, 3,5-dimethyl-4-(methylsulfinyl)-, methylcarbamate
	Carbamic acid, methyl-, 4-(methylsulfinyl)-3,5-xylyl ester
	Bay 37344 sulfoxide
	BAY 41791
	4-(Methylsulfinyl)-3,5-xylyl methylcarbamate
	BAYER 41791
	Carbamic acid, methyl-, 3,5-dimethyl-4-(methylsulfinyl)phenyl ester
	3,5-Dimethyl-4-(methylsulfinyl)phenyl methylcarbamate
	ENT 25824
	Methiocarb sulfoxide
	Phenol, 3,5-dimethyl-4-(methylsulfinyl)-, (N-methylcarbamate)
Inchi:	InChI=1S/C11H15NO3S/c1-7-5-9(15-11(13)12-3)6-8(2)10(7)16(4)14/h5-6H,1-4H3,(H,12,
InchiKey:	FNCMBMZOZQAWJA-UHFFFAOYSA-N
Formula:	C11H15NO3S
SMILES:	CNC(=O)Oc1cc(C)c(S(C)=O)c(C)c1
Mol. weight [g/mol]:	241.31
CAS:	2635-10-1

Physical Properties

Property code	Value	Unit	Source
gf	-236.98	kJ/mol	Joback Method
hf	-465.32	kJ/mol	Joback Method
hfus	32.76	kJ/mol	Joback Method
hvap	72.66	kJ/mol	Joback Method
log10ws	-2.40		Crippen Method
logp	1.759		Crippen Method
mcvol	181.730	ml/mol	McGowan Method
pc	2944.08	kPa	Joback Method
tb	677.44	K	Joback Method
tc	893.43	K	Joback Method
tf	439.01	K	Joback Method
vc	0.693	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	462.44	J/mol×K	677.44	Joback Method
cpg	475.87	J/mol×K	713.44	Joback Method
cpg	488.44	J/mol×K	749.44	Joback Method
cpg	500.15	J/mol×K	785.44	Joback Method
cpg	510.97	J/mol×K	821.44	Joback Method
cpg	520.92	J/mol×K	857.44	Joback Method
cpg	529.98	J/mol×K	893.43	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2635101&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume