

Sulfoxide

Other names:

1,3-Benzodioxole, 5-[2-(octylsulfinyl)propyl]-
Benzene, 1,2-(methylenedioxy)-4-[2-(octylsulfinyl)propyl]-
n-Octylisosafole sulfoxide
Isosafole n-octylsulfoxide
Isosafole octyl sulfoxide
Piperonyl sulfoxide
Sulfox-cide
Sulfoxide, «alpha»-methyl-3,4-(methylenedioxy)phenethyl octyl
Sulfoxyl
Sulphoxide
1-Methyl-2-(3,4-methylenedioxyphenyl)ethyl octyl sulfoxide
1,2-(Methylenedioxy)-4-[2-(octylsulfinyl)propyl]benzene
1,2-Methoxylenedioxy-4-[2-(octylsulfinyl)propyl]benzene
5-[2-(Octylsulfinyl)propyl]-1,3-benzodioxole
n-Octylsulfoxide of isosafole
ENT 16,634
NCI-C02824
1-(2,3-Methylendioxyfenyl)-2-(oktylsufinyl)propan
Sulfocide
NSC 8400
Piperonyl sulfoxide (insecticide)
Sulfoxide (synergist)
1-(3,4-methylenedioxyphenyl)isopropyl octyl sulphoxide

Inchi: InChI=1S/C18H28O3S/c1-3-4-5-6-7-8-11-22(19)15(2)12-16-9-10-17-18(13-16)21-14-20-

InchiKey: ATTZFSUZZUNHBP-UHFFFAOYSA-N

Formula: C18H28O3S

SMILES: CCCCCCCCS(=O)C(C)Cc1ccc2c(c1)OCO2

Mol. weight [g/mol]: 324.48

CAS: 120-62-7

Physical Properties

Property code	Value	Unit	Source
gf	-130.10	kJ/mol	Joback Method
hf	-583.14	kJ/mol	Joback Method
hfus	52.89	kJ/mol	Joback Method
hvap	80.84	kJ/mol	Joback Method

log10ws	-5.00		Crippen Method
logp	4.456		Crippen Method
mcvol	263.820	ml/mol	McGowan Method
pc	1727.46	kPa	Joback Method
tb	771.03	K	Joback Method
tc	975.86	K	Joback Method
tf	440.88	K	Joback Method
vc	1.020	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	787.50	J/mol×K	771.03	Joback Method
cpg	804.70	J/mol×K	805.17	Joback Method
cpg	820.82	J/mol×K	839.31	Joback Method
cpg	835.92	J/mol×K	873.44	Joback Method
cpg	850.05	J/mol×K	907.58	Joback Method
cpg	863.28	J/mol×K	941.72	Joback Method
cpg	875.66	J/mol×K	975.86	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C120627&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

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

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