

6-ethoxy-2-(6-ethoxy-3-oxobenzo[b]thien-2(3H)-ylidene)benzo[b]thiophen-3(2H)-one

Other names:

Inchi:	6-Ethoxy-2-(6-ethoxy-3-oxobenzo[b]thien-2(3H)-ylidene)benzo[b]thiophen-3(2H)-one (C.I. Vat Orange 5)
InchiKey:	VMXWZRNWXZSSCE-FMQUCBEESA-N
Formula:	C20H16O4S2
SMILES:	CCOc1ccc2c(c1)SC(=C1Sc3cc(OCC)ccc3C1=O)C2=O
Mol. weight [g/mol]:	384.47
CAS:	3263-31-8

Physical Properties

Property code	Value	Unit	Source
gf	75.98	kJ/mol	Joback Method
hf	-257.15	kJ/mol	Joback Method
hfus	37.36	kJ/mol	Joback Method
hvap	94.31	kJ/mol	Joback Method
log10ws	-6.80		Crippen Method
logp	4.973		Crippen Method
mcvol	266.700	ml/mol	McGowan Method
pc	2104.20	kPa	Joback Method
tb	1038.36	K	Joback Method
tc	1311.69	K	Joback Method
tf	836.04	K	Joback Method
vc	0.984	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	808.89	J/molxK	1038.36	Joback Method
cpg	819.65	J/molxK	1083.91	Joback Method
cpg	828.90	J/molxK	1129.47	Joback Method
cpg	836.67	J/molxK	1175.02	Joback Method
cpg	843.02	J/molxK	1220.58	Joback Method
cpg	847.97	J/molxK	1266.13	Joback Method
cpg	851.57	J/molxK	1311.69	Joback Method
hsubt	65.00	kJ/mol	576.50	NIST Webbook

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=C3263318&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
hsubt:	Enthalpy of sublimation at a given temperature
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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