(2E)-1,3-bis(4-ethoxyphenyl)-2-buten-1-one

Inchi: InChI=1S/C20H22O3/c1-4-22-18-10-6-16(7-11-18)15(3)14-20(21)17-8-12-19(13-9-17)23
InchiKey: SSRURNGOFBSAOS-CCEZHUSRSA-N
Formula: C20H22O3
SMILES: CCOc1ccc(C(=O)C=C(C)c2ccc(OCC)cc2)cc1
Mol. weight [g/mol]: 310.39
CAS: 116373-31-0

Physical Properties

Property code	Value	Unit	Source
gf	55.83	kJ/mol	Joback Method
hf	-275.60	kJ/mol	Joback Method
hfus	37.73	kJ/mol	Joback Method
hvap	77.59	kJ/mol	Joback Method
log10ws	-5.68		Crippen Method
logp	4.770		Crippen Method
mcvol	254.150	ml/mol	McGowan Method
pc	1707.53	kPa	Joback Method
tb	823.07	K	Joback Method
tc	1050.95	K	Joback Method
tf	468.39	K	Joback Method
vc	0.963	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	739.23	J/mol×K	823.07	Joback Method
cpg	755.13	J/mol×K	861.05	Joback Method
cpg	769.80	J/mol×K	899.03	Joback Method
cpg	783.29	J/mol×K	937.01	Joback Method
cpg	795.64	J/mol×K	974.99	Joback Method
cpg	806.91	J/mol×K	1012.97	Joback Method
cpg	817.16	J/mol×K	1050.95	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=C116373310&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume