Benzoic acid, p-(alpha-ethoxy-p-phenylphenacylamino)-

Inchi: InChI=1S/C23H21NO4/c1-2-28-22(24-20-14-12-19(13-15-20)23(26)27)21(25)18-10-8-17

InchiKey: BPOMPTVRBWXZBY-UHFFFAOYSA-N

Formula: C23H21NO4

SMILES: CCOC(Nc1ccc(C(=O)O)cc1)C(=O)c1ccc(-c2ccccc2)cc1

Mol. weight [g/mol]: 375.42

CAS: 1174-11-4

Physical Properties

Property code	Value	Unit	Source
gf	48.04	kJ/mol	Joback Method
hf	-292.82	kJ/mol	Joback Method
hfus	46.72	kJ/mol	Joback Method
hvap	113.57	kJ/mol	Joback Method
log10ws	-6.57		Crippen Method
logp	4.709		Crippen Method
mcvol	288.510	ml/mol	McGowan Method
pc	1991.21	kPa	Joback Method
tb	1087.71	K	Joback Method
tc	1337.28	K	Joback Method
tf	673.84	K	Joback Method
vc	1.077	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	919.93	J/mol×K	1087.71	Joback Method
cpg	928.91	J/mol×K	1129.31	Joback Method
cpg	936.78	J/mol×K	1170.90	Joback Method
cpg	943.65	J/mol×K	1212.50	Joback Method
cpg	949.60	J/mol×K	1254.09	Joback Method
cpg	954.75	J/mol×K	1295.69	Joback Method
cpg	959.20	J/mol×K	1337.28	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=C1174114&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