4-Ethylbenzoic acid, 2,6-dimethylnon-1-en-3-yn-5-yl ester

Inchi: InChI=1S/C20H26O2/c1-6-8-16(5)19(14-9-15(3)4)22-20(21)18-12-10-17(7-2)11-13-18/h1

InchiKey: RCCWFOTWJIIRJG-UHFFFAOYSA-N

Formula: C20H26O2

SMILES: C=C(C)C#CC(OC(=O)c1ccc(CC)cc1)C(C)CCC

Mol. weight [g/mol]: 298.42

Physical Properties

Property code	Value	Unit	Source
gf	263.59	kJ/mol	Joback Method
hf	-98.49	kJ/mol	Joback Method
hfus	37.48	kJ/mol	Joback Method
hvap	72.99	kJ/mol	Joback Method
log10ws	-6.22		Crippen Method
logp	4.790		Crippen Method
mcvol	263.440	ml/mol	McGowan Method
pc	1534.26	kPa	Joback Method
rinpol	2087.80		NIST Webbook
tb	769.63	K	Joback Method
tc	987.46	K	Joback Method
tf	486.64	K	Joback Method
vc	1.004	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	753.20	J/mol×K	769.63	Joback Method
cpg	771.17	J/mol×K	805.94	Joback Method
cpg	787.96	J/mol×K	842.24	Joback Method
cpg	803.61	J/mol×K	878.55	Joback Method
cpg	818.16	J/mol×K	914.85	Joback Method
cpg	831.67	J/mol×K	951.16	Joback Method
cpg	844.18	J/mol×K	987.46	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=U292547&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume