4-Ethylbenzoic acid, tridec-2-ynyl ester

Inchi: InChI=1S/C22H32O2/c1-3-5-6-7-8-9-10-11-12-13-14-19-24-22(23)21-17-15-20(4-2)16-18
InchiKey: PUNWFZUZTKEVJC-UHFFFAOYSA-N
Formula: C22H32O2
SMILES: CCCCCCCCCCC#CCOC(=O)c1ccc(CC)cc1
Mol. weight [g/mol]: 328.49

Physical Properties

Property code	Value	Unit	Source
gf	206.02	kJ/mol	Joback Method
hf	-244.85	kJ/mol	Joback Method
hfus	52.30	kJ/mol	Joback Method
hvap	78.81	kJ/mol	Joback Method
log10ws	-7.33		Crippen Method
logp	5.940		Crippen Method
mcvol	295.920	ml/mol	McGowan Method
pc	1268.25	kPa	Joback Method
rinpol	2527.10		NIST Webbook
tb	819.71	K	Joback Method
tc	1023.51	K	Joback Method
tf	554.90	K	Joback Method
vc	1.145	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	895.64	J/mol×K	819.71	Joback Method
cpg	913.71	J/mol×K	853.68	Joback Method
cpg	930.66	J/mol×K	887.64	Joback Method
cpg	946.51	J/mol×K	921.61	Joback Method
cpg	961.32	J/mol×K	955.58	Joback Method
cpg	975.11	J/mol×K	989.54	Joback Method
cpg	987.93	J/mol×K	1023.51	Joback Method

Sources

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=U292549&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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