4-Ethylbenzoic acid, dodec-9-ynyl ester

Inchi: InChI=1S/C21H30O2/c1-3-5-6-7-8-9-10-11-12-13-18-23-21(22)20-16-14-19(4-2)15-17-20
InchiKey: KAZMWHCOWVPOMU-UHFFFAOYSA-N
Formula: C21H30O2
SMILES: CCC#CCCCCCCCCOC(=O)c1ccc(CC)cc1
Mol. weight [g/mol]: 314.46

Physical Properties

Property code	Value	Unit	Source
gf	197.60	kJ/mol	Joback Method
hf	-224.21	kJ/mol	Joback Method
hfus	49.71	kJ/mol	Joback Method
hvap	76.59	kJ/mol	Joback Method
log10ws	-6.92		Crippen Method
logp	5.550		Crippen Method
mcvol	281.830	ml/mol	McGowan Method
pc	1359.63	kPa	Joback Method
rinpol	2460.30		NIST Webbook
rinpol	2460.30		NIST Webbook
tb	796.83	K	Joback Method
tc	1001.35	K	Joback Method
tf	543.63	K	Joback Method
vc	1.089	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	836.53	J/mol×K	796.83	Joback Method
cpg	854.43	J/mol×K	830.92	Joback Method
cpg	871.22	J/mol×K	865.00	Joback Method
cpg	886.94	J/mol×K	899.09	Joback Method
cpg	901.63	J/mol×K	933.18	Joback Method
cpg	915.32	J/mol×K	967.27	Joback Method
cpg	928.06	J/mol×K	1001.35	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292202&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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