4-Ethylbenzoic acid, nonyl ester

Inchi: InChI=1S/C18H28O2/c1-3-5-6-7-8-9-10-15-20-18(19)17-13-11-16(4-2)12-14-17/h11-14H
InchiKey: KIRYMGVAUXIGQJ-UHFFFAOYSA-N
Formula: C18H28O2
SMILES: CCCCCCCCCOC(=O)c1ccc(CC)cc1
Mol. weight [g/mol]: 276.41

Physical Properties

Property code	Value	Unit	Source
gf	-30.46	kJ/mol	Joback Method
hf	-434.59	kJ/mol	Joback Method
hfus	38.81	kJ/mol	Joback Method
hvap	67.76	kJ/mol	Joback Method
log10ws	-5.87		Crippen Method
logp	5.156		Crippen Method
mcvol	248.160	ml/mol	McGowan Method
pc	1497.67	kPa	Joback Method
rinpol	2114.40		NIST Webbook
rinpol	2114.40		NIST Webbook
tb	719.19	K	Joback Method
tc	912.00	K	Joback Method
tf	403.72	K	Joback Method
vc	0.960	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.68	J/mol×K	719.19	Joback Method
cpg	789.43	J/mol×K	879.87	Joback Method
cpg	775.53	J/mol×K	847.73	Joback Method
cpg	760.73	J/mol×K	815.60	Joback Method
cpg	745.01	J/mol×K	783.46	Joback Method
cpg	728.33	J/mol×K	751.33	Joback Method
cpg	802.46	J/mol×K	912.00	Joback Method
dvisc	0.0000958	Pa×s	719.19	Joback Method

dvisc	0.0001240	Pa×s	666.61	Joback Method
dvisc	0.0001678	Pa×s	614.03	Joback Method
dvisc	0.0002404	Pa×s	561.46	Joback Method
dvisc	0.0003708	Pa×s	508.88	Joback Method
dvisc	0.0006322	Pa×s	456.30	Joback Method
dvisc	0.0012384	Pa×s	403.72	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=U292197&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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