4-Ethylbenzoic acid, oct-3-en-2-yl ester

Inchi: InChI=1S/C17H24O2/c1-4-6-7-8-9-14(3)19-17(18)16-12-10-15(5-2)11-13-16/h8-14H,4-7H
InchiKey: YUYNJMYTXVXSKB-CMDGGOBGSA-N
Formula: C17H24O2
SMILES: CCCCC=CC(C)OC(=O)c1ccc(CC)cc1
Mol. weight [g/mol]: 260.37

Physical Properties

Property code	Value	Unit	Source
gf	38.90	kJ/mol	Joback Method
hf	-302.01	kJ/mol	Joback Method
hfus	32.90	kJ/mol	Joback Method
hvap	65.10	kJ/mol	Joback Method
log10ws	-5.41		Crippen Method
logp	4.541		Crippen Method
mcvol	229.770	ml/mol	McGowan Method
pc	1696.30	kPa	Joback Method
rinpol	1917.20		NIST Webbook
rinpol	1917.20		NIST Webbook
tb	700.03	K	Joback Method
tc	904.10	K	Joback Method
tf	372.37	K	Joback Method
vc	0.877	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	632.39	J/mol×K	700.03	Joback Method
cpg	649.57	J/mol×K	734.04	Joback Method
cpg	665.75	J/mol×K	768.05	Joback Method
cpg	680.95	J/mol×K	802.06	Joback Method
cpg	695.22	J/mol×K	836.07	Joback Method
cpg	708.61	J/mol×K	870.08	Joback Method
cpg	721.14	J/mol×K	904.10	Joback Method
dvisc	0.0015056	Pa×s	372.37	Joback Method

dvisc	0.0006890	Pa×s	426.98	Joback Method
dvisc	0.0003765	Pa×s	481.59	Joback Method
dvisc	0.0002327	Pa×s	536.20	Joback Method
dvisc	0.0001572	Pa×s	590.81	Joback Method
dvisc	0.0001135	Pa×s	645.42	Joback Method
dvisc	0.0000862	Pa×s	700.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292544&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
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