4-Ethylbenzoic acid, octyl ester

Inchi: InChI=1S/C17H26O2/c1-3-5-6-7-8-9-14-19-17(18)16-12-10-15(4-2)11-13-16/h10-13H,3-9
InchiKey: PXGCAPRMDJWYHP-UHFFFAOYSA-N
Formula: C17H26O2
SMILES: CCCCCCCCOC(=O)c1ccc(CC)cc1
Mol. weight [g/mol]: 262.39

Physical Properties

Property code	Value	Unit	Source
gf	-38.88	kJ/mol	Joback Method
hf	-413.95	kJ/mol	Joback Method
hfus	36.23	kJ/mol	Joback Method
hvap	65.53	kJ/mol	Joback Method
log10ws	-5.45		Crippen Method
logp	4.766		Crippen Method
mcvol	234.070	ml/mol	McGowan Method
pc	1615.47	kPa	Joback Method
rinpol	2006.60		NIST Webbook
rinpol	2006.60		NIST Webbook
tb	696.31	K	Joback Method
tc	890.56	K	Joback Method
tf	392.45	K	Joback Method
vc	0.903	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	654.61	J/mol×K	696.31	Joback Method
cpg	671.96	J/mol×K	728.69	Joback Method
cpg	688.36	J/mol×K	761.06	Joback Method
cpg	703.83	J/mol×K	793.44	Joback Method
cpg	718.39	J/mol×K	825.81	Joback Method
cpg	732.07	J/mol×K	858.19	Joback Method
cpg	744.91	J/mol×K	890.56	Joback Method
dvisc	0.0013343	Pa×s	392.45	Joback Method

dvisc	0.0006905	Pa×s	443.09	Joback Method
dvisc	0.0004091	Pa×s	493.74	Joback Method
dvisc	0.0002671	Pa×s	544.38	Joback Method
dvisc	0.0001876	Pa×s	595.02	Joback Method
dvisc	0.0001392	Pa×s	645.67	Joback Method
dvisc	0.0001079	Pa×s	696.31	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=U292345&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
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