2-Ethylhexyl 3,4-dimethylbenzoate

Inchi: InChI=1S/C17H26O2/c1-5-7-8-15(6-2)12-19-17(18)16-10-9-13(3)14(4)11-16/h9-11,15H,5
InchiKey: NOJFKUNHDNKRPS-UHFFFAOYSA-N
Formula: C17H26O2
SMILES: CCCCC(CC)COC(=O)c1ccc(C)c(C)c1
Mol. weight [g/mol]: 262.39

Physical Properties

Property code	Value	Unit	Source
gf	-50.95	kJ/mol	Joback Method
hf	-430.70	kJ/mol	Joback Method
hfus	32.31	kJ/mol	Joback Method
hvap	65.80	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	4.677		Crippen Method
mcvol	234.070	ml/mol	McGowan Method
pc	1606.42	kPa	Joback Method
rinpol	1920.00		NIST Webbook
tb	700.85	K	Joback Method
tc	898.99	K	Joback Method
tf	389.97	K	Joback Method
vc	0.897	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	654.79	J/mol×K	700.85	Joback Method
cpg	672.31	J/mol×K	733.87	Joback Method
cpg	688.85	J/mol×K	766.90	Joback Method
cpg	704.44	J/mol×K	799.92	Joback Method
cpg	719.10	J/mol×K	832.94	Joback Method
cpg	732.85	J/mol×K	865.97	Joback Method
cpg	745.72	J/mol×K	898.99	Joback Method
dvisc	0.0012847	Pa×s	389.97	Joback Method
dvisc	0.0006534	Pa×s	441.78	Joback Method

dvisc	0.0003830	Pa×s	493.60	Joback Method
dvisc	0.0002485	Pa×s	545.41	Joback Method
dvisc	0.0001738	Pa×s	597.22	Joback Method
dvisc	0.0001287	Pa×s	649.04	Joback Method
dvisc	0.0000996	Pa×s	700.85	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=R540326&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