2-Ethylhexyl 2-phenoxypropionate

Inchi: InChI=1S/C17H26O3/c1-4-6-10-15(5-2)13-19-17(18)14(3)20-16-11-8-7-9-12-16/h7-9,11-
InchiKey: KKSYEZLSHKWXEN-UHFFFAOYSA-N
Formula: C17H26O3
SMILES: CCCCC(CC)COC(=O)C(C)Oc1ccccc1
Mol. weight [g/mol]: 278.39

Physical Properties

Property code	Value	Unit	Source
gf	-139.13	kJ/mol	Joback Method
hf	-545.26	kJ/mol	Joback Method
hfus	30.76	kJ/mol	Joback Method
hvap	66.50	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	4.214		Crippen Method
mcvol	239.940	ml/mol	McGowan Method
pc	1633.81	kPa	Joback Method
rinpol	1803.00		NIST Webbook
tb	712.87	K	Joback Method
tc	911.35	K	Joback Method
tf	372.16	K	Joback Method
vc	0.909	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	685.13	J/mol×K	712.87	Joback Method
cpg	702.79	J/mol×K	745.95	Joback Method
cpg	719.41	J/mol×K	779.03	Joback Method
cpg	734.99	J/mol×K	812.11	Joback Method
cpg	749.56	J/mol×K	845.19	Joback Method
cpg	763.14	J/mol×K	878.27	Joback Method
cpg	775.76	J/mol×K	911.35	Joback Method
dvisc	0.0017910	Pa×s	372.16	Joback Method
dvisc	0.0007332	Pa×s	428.94	Joback Method

dvisc	0.0003699	Pa×s	485.73	Joback Method
dvisc	0.0002153	Pa×s	542.51	Joback Method
dvisc	0.0001389	Pa×s	599.30	Joback Method
dvisc	0.0000967	Pa×s	656.09	Joback Method
dvisc	0.0000713	Pa×s	712.87	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R540311&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

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