2-Ethylhexyl 2-phenoxybenzoate

Inchi: InChI=1S/C21H26O3/c1-3-5-11-17(4-2)16-23-21(22)19-14-9-10-15-20(19)24-18-12-7-6-8
InchiKey: MFXGMWHXGXQNKD-UHFFFAOYSA-N
Formula: C21H26O3
SMILES: CCCCC(CC)COC(=O)c1ccccc1Oc1ccccc1
Mol. weight [g/mol]: 326.43

Physical Properties

Property code	Value	Unit	Source
gf	-0.23	kJ/mol	Joback Method
hf	-397.48	kJ/mol	Joback Method
hfus	38.29	kJ/mol	Joback Method
hvap	78.73	kJ/mol	Joback Method
log10ws	-6.04		Crippen Method
logp	5.852		Crippen Method
mcvol	272.540	ml/mol	McGowan Method
pc	1537.87	kPa	Joback Method
rinpol	2256.00		NIST Webbook
tb	836.49	K	Joback Method
tc	1055.17	K	Joback Method
tf	471.18	K	Joback Method
vc	1.032	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	824.97	J/mol×K	836.49	Joback Method
cpg	841.52	J/mol×K	872.94	Joback Method
cpg	856.75	J/mol×K	909.38	Joback Method
cpg	870.72	J/mol×K	945.83	Joback Method
cpg	883.45	J/mol×K	982.28	Joback Method
cpg	894.99	J/mol×K	1018.73	Joback Method
cpg	905.39	J/mol×K	1055.17	Joback Method
dvisc	0.0006399	Pa×s	471.18	Joback Method
dvisc	0.0003217	Pa×s	532.07	Joback Method

dvisc	0.0001863	Pa×s	592.95	Joback Method
dvisc	0.0001194	Pa×s	653.84	Joback Method
dvisc	0.0000826	Pa×s	714.72	Joback Method
dvisc	0.0000605	Pa×s	775.61	Joback Method
dvisc	0.0000464	Pa×s	836.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R540297&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

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