Mono(2-ethylhexyl) phthalate

Other names:	1,2-Benzenedicarboxylic acid, mono(2-ethylhexyl) ester
	Phthalic acid, mono-(2-ethylhexyl) ester
	Mehp
	Monoethylhexyl phthalate
	2-((2-Ethylhexyloxy)carbonyl)benzoic acid
	(2-ethylhexyl) hydrogen phthalate
Inchi:	InChI=1S/C16H22O4/c1-3-5-8-12(4-2)11-20-16(19)14-10-7-6-9-13(14)15(17)18/h6-7,9-1
InchiKey:	DJDSLBVSSOQSLW-UHFFFAOYSA-N
Formula:	C16H22O4
SMILES:	CCCCC(CC)COC(=O)c1ccccc1C(=O)O
Mol. weight [g/mol]:	278.34
CAS:	4376-20-9

Physical Properties

Property code	Value	Unit	Source
gf	-315.48	kJ/mol	Joback Method
hf	-663.40	kJ/mol	Joback Method
hfus	35.80	kJ/mol	Joback Method
hvap	86.34	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	3.758		Crippen Method
mcvol	227.420	ml/mol	McGowan Method
pc	2012.70	kPa	Joback Method
rinpol	2152.00		NIST Webbook
rinpol	2152.00		NIST Webbook
tb	819.04	K	Joback Method
tc	1019.27	K	Joback Method
tf	476.93	K	Joback Method
vc	0.867	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	679.33	J/mol×K	819.04	Joback Method

cpg	692.23	J/mol×K	852.41	Joback Method
cpg	704.24	J/mol×K	885.78	Joback Method
cpg	715.38	J/mol×K	919.15	Joback Method
cpg	725.69	J/mol×K	952.52	Joback Method
cpg	735.19	J/mol×K	985.90	Joback Method
cpg	743.90	J/mol×K	1019.27	Joback Method
dvisc	0.0007462	Pa×s	476.93	Joback Method
dvisc	0.0002933	Pa×s	533.95	Joback Method
dvisc	0.0001380	Pa×s	590.97	Joback Method
dvisc	0.0000742	Pa×s	647.99	Joback Method
dvisc	0.0000441	Pa×s	705.00	Joback Method
dvisc	0.0000283	Pa×s	762.02	Joback Method
dvisc	0.0000193	Pa×s	819.04	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4376209&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