1,2-Benzenedicarboxylic acid, mono(2-ethylhexyl) ester

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]: 278.35

Physical Properties

Property code	Value	Unit	Source
af	0.9694		Cheméo Relay (1.0)
hf	-773.01	kJ/mol	Cheméo Relay (1.0)
hfus	35.80	kJ/mol	Joback Method
hvap	108.18	kJ/mol	Cheméo Relay (1.0)
log10ws	-4.36		Cheméo Relay (1.0)
logp	3.758		Crippen Method
mcvol	227.420	ml/mol	McGowan Method
pc	2012.70	kPa	Joback Method
tb	616.17	K	Cheméo Relay (1.0)
tc	847.21	K	Cheméo Relay (1.0)
tf	308.89	K	Cheméo Relay (1.0)
vc	0.808	m3/kmol	Cheméo Relay (1.0)

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

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4376209&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume