BENZENACETIC ACID, 3-ETHOXY-4-HYDROXY-

Other names: Benzenacetic acid, 3-ethoxy-4-hydroxy-
Benzeneacetic acid, 3-ethoxy-4-hydroxy-
Inchi: InChI=1S/C10H12O4/c1-2-14-9-5-7(6-10(12)13)3-4-8(9)11/h3-5,11H,2,6H2,1H3,(H,12,13
InchiKey: QVXSHYZATYQYGE-UHFFFAOYSA-N
Formula: C10H12O4
SMILES: CCOc1cc(CC(=O)O)ccc1O
Mol. weight [g/mol]: 196.20

Physical Properties

Property code	Value	Unit	Source
hfus	27.97	kJ/mol	Joback Method
ie	7.89	eV	Cheméo Relay (1.0)
log10ws	-1.66		Cheméo Relay (1.0)
logp	1.418		Crippen Method
mcvol	147.180	ml/mol	McGowan Method
tb	576.25	K	Cheméo Relay (1.0)
tf	398.37	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.98	J/mol×K	708.95	Joback Method
cpg	404.64	J/mol×K	743.72	Joback Method
cpg	413.76	J/mol×K	778.50	Joback Method
cpg	422.39	J/mol×K	813.27	Joback Method
cpg	430.57	J/mol×K	848.04	Joback Method
cpg	438.35	J/mol×K	882.82	Joback Method
cpg	445.79	J/mol×K	917.59	Joback Method
dvisc	0.0002007	Pa×s	486.10	Joback Method
dvisc	0.0000856	Pa×s	523.24	Joback Method
dvisc	0.0000409	Pa×s	560.38	Joback Method
dvisc	0.0000214	Pa×s	597.53	Joback Method
dvisc	0.0000121	Pa×s	634.67	Joback Method
dvisc	0.0000073	Pa×s	671.81	Joback Method

dvisc	0.0000046	Pa×s	708.95	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C80018504&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

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hfus: Enthalpy of fusion at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point

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