3-Ethoxy-4-hydroxyphenylacetic acid

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
CAS: 80018-50-4

Physical Properties

Property code	Value	Unit	Source
gf	-389.26	kJ/mol	Joback Method
hf	-599.01	kJ/mol	Joback Method
hfus	27.97	kJ/mol	Joback Method
hvap	79.64	kJ/mol	Joback Method
log10ws	-1.46		Crippen Method
logp	1.418		Crippen Method
mcvol	147.180	ml/mol	McGowan Method
pc	4031.24	kPa	Joback Method
tb	708.95	K	Joback Method
tc	917.59	K	Joback Method
tf	486.10	K	Joback Method
vc	0.496	m3/kmol	Joback Method

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	597.52	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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C80018504&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume