(4-Ethyl-phenoxy)-acetic acid

Other names: Acetic acid, (4-ethylphenoxy)-
Inchi: InChI=1S/C10H12O3/c1-2-8-3-5-9(6-4-8)13-7-10(11)12/h3-6H,2,7H2,1H3,(H,11,12)
InchiKey: WVELHLIHMYYZAT-UHFFFAOYSA-N
Formula: C10H12O3
SMILES: CCc1ccc(OCC(=O)O)cc1
Mol. weight [g/mol]: 180.20

Physical Properties

Property code	Value	Unit	Source
af	0.7649		Cheméo Relay (1.0)
hf	-492.75	kJ/mol	Cheméo Relay (1.0)
hfus	22.18	kJ/mol	Joback Method
hvap	84.54	kJ/mol	Cheméo Relay (1.0)
ie	8.27	eV	Cheméo Relay (1.0)
log10ws	-2.30		Cheméo Relay (1.0)
logp	1.712		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	3364.54	kPa	Joback Method
tb	568.84	K	Cheméo Relay (1.0)
tc	777.86	K	Cheméo Relay (1.0)
tf	365.06	K	Cheméo Relay (1.0)
vc	0.508	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.22	J/mol×K	628.33	Joback Method
cpg	406.96	J/mol×K	827.77	Joback Method
cpg	398.96	J/mol×K	794.53	Joback Method
cpg	390.39	J/mol×K	761.29	Joback Method
cpg	381.24	J/mol×K	728.05	Joback Method
cpg	371.50	J/mol×K	694.81	Joback Method
cpg	361.17	J/mol×K	661.57	Joback Method
dvisc	0.0002546	Pa×s	501.35	Joback Method

dvisc	0.0000667	Pa×s	628.33	Joback Method
dvisc	0.0000978	Pa×s	586.00	Joback Method
dvisc	0.0001520	Pa×s	543.68	Joback Method
dvisc	0.0024094	Pa×s	374.38	Joback Method
dvisc	0.0004691	Pa×s	459.03	Joback Method
dvisc	0.0009783	Pa×s	416.70	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C24431274&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

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
ie: Ionization energy
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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.