

4-Ethoxyphenylacetic acid

Other names:	para-Ethoxyphenylacetic acid 4-Ethoxyphenylacetic acid p-Ethoxyphenylacetic acid
Inchi:	InChI=1S/C10H12O3/c1-2-13-9-5-3-8(4-6-9)7-10(11)12/h3-6H,2,7H2,1H3,(H,11,12)
InchiKey:	ZVWZNFMSMIFGEP-UHFFFAOYSA-N
Formula:	C10H12O3
SMILES:	CCOc1ccc(CC(=O)O)cc1
Mol. weight [g/mol]:	180.20

Physical Properties

Property code	Value	Unit	Source
af	0.7534		Cheméo Relay (1.0)
hf	-511.31	kJ/mol	Cheméo Relay (1.0)
hfus	22.18	kJ/mol	Joback Method
hvap	84.12	kJ/mol	Cheméo Relay (1.0)
ie	8.03	eV	Cheméo Relay (1.0)
log10ws	-2.15		Cheméo Relay (1.0)
logp	1.712		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	3364.54	kPa	Joback Method
tb	576.93	K	Cheméo Relay (1.0)
tc	774.77	K	Cheméo Relay (1.0)
tf	360.00 ± 0.50	K	NIST Webbook

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	0.0001520	Pa×s	543.68	Joback Method
dvisc	0.0000667	Pa×s	628.33	Joback Method
dvisc	0.0000978	Pa×s	586.00	Joback Method
dvisc	0.0024094	Pa×s	374.38	Joback Method
dvisc	0.0002546	Pa×s	501.35	Joback Method
dvisc	0.0004691	Pa×s	459.03	Joback Method
dvisc	0.0009783	Pa×s	416.70	Joback Method
hfust	23.00	kJ/mol	360.20	NIST Webbook
hfust	23.00	kJ/mol	360.20	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C4919339&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
hfust:	Enthalpy of fusion at a given temperature
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

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