

(4-Tert-butylphenoxy)acetic acid

Inchi:	InChI=1S/C12H16O3/c1-12(2,3)9-4-6-10(7-5-9)15-8-11(13)14/h4-7H,8H2,1-3H3,(H,13,14)
InchiKey:	FBIGAJNVRFKBJL-UHFFFAOYSA-N
Formula:	C12H16O3
SMILES:	CC(C)(C)c1ccc(OCC(=O)O)cc1
Mol. weight [g/mol]:	208.25
CAS:	1798-04-5

Physical Properties

Property code	Value	Unit	Source
gf	-214.96	kJ/mol	Joback Method
hf	-471.73	kJ/mol	Joback Method
hfus	19.95	kJ/mol	Joback Method
hvap	69.78	kJ/mol	Joback Method
log10ws	-2.42		Crippen Method
logp	2.447		Crippen Method
mcvol	169.490	ml/mol	McGowan Method
pc	2778.85	kPa	Joback Method
tb	670.86	K	Joback Method
tc	875.23	K	Joback Method
tf	399.34	K	Joback Method
vc	0.631	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	452.32	J/molxK	670.86	Joback Method
cpg	464.97	J/molxK	704.92	Joback Method
cpg	476.81	J/molxK	738.98	Joback Method
cpg	487.87	J/molxK	773.04	Joback Method
cpg	498.20	J/molxK	807.11	Joback Method
cpg	507.83	J/molxK	841.17	Joback Method
cpg	516.79	J/molxK	875.23	Joback Method
dvisc	0.0018429	Paxs	399.34	Joback Method
dvisc	0.0007084	Paxs	444.59	Joback Method

dvisc	0.0003249	Paxs	489.85	Joback Method
dvisc	0.0001700	Paxs	535.10	Joback Method
dvisc	0.0000984	Paxs	580.35	Joback Method
dvisc	0.0000617	Paxs	625.61	Joback Method
dvisc	0.0000412	Paxs	670.86	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1798045&Units=SI

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

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