(3-methylphenoxy)acetic acid

Inchi: InChI=1S/C9H10O3/c1-7-3-2-4-8(5-7)12-6-9(10)11/h2-5H,6H2,1H3,(H,10,11)
InchiKey: VZECTCSEONQIPP-UHFFFAOYSA-N
Formula: C9H10O3
SMILES: Cc1cccc(OCC(=O)O)c1
Mol. weight [g/mol]: 166.17
CAS: 1643-15-8

Physical Properties

Property code	Value	Unit	Source
gf	-243.06	kJ/mol	Joback Method
hf	-401.06	kJ/mol	Joback Method
hfus	19.59	kJ/mol	Joback Method
hvap	64.40	kJ/mol	Joback Method
log10ws	-1.58		Crippen Method
logp	1.458		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
pc	3773.04	kPa	Joback Method
tb	605.45	K	Joback Method
tc	807.67	K	Joback Method
tf	363.11	K	Joback Method
vc	0.474	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.01	J/mol×K	605.45	Joback Method
cpg	313.16	J/mol×K	639.15	Joback Method
cpg	322.74	J/mol×K	672.86	Joback Method
cpg	331.76	J/mol×K	706.56	Joback Method
cpg	340.24	J/mol×K	740.27	Joback Method
cpg	348.17	J/mol×K	773.97	Joback Method
cpg	355.59	J/mol×K	807.67	Joback Method
dvisc	0.0027550	Pa×s	363.11	Joback Method
dvisc	0.0011315	Pa×s	403.50	Joback Method

dvisc	0.0005464	Pa×s	443.89	Joback Method
dvisc	0.0002980	Pa×s	484.28	Joback Method
dvisc	0.0001784	Pa×s	524.67	Joback Method
dvisc	0.0001149	Pa×s	565.06	Joback Method
dvisc	0.0000785	Pa×s	605.45	Joback Method

Sources

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=C1643158&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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