2-(4-Formylphenyl)propanoic acid, methyl

Inchi: InChI=1S/C11H12O3/c1-8(11(13)14-2)10-5-3-9(7-12)4-6-10/h3-8H,1-2H3
InchiKey: RBAQUIFHFPBFJL-UHFFFAOYSA-N
Formula: C11H12O3
SMILES: COC(=O)C(C)c1ccc(C=O)cc1
Mol. weight [g/mol]: 192.21

Physical Properties

Property code	Value	Unit	Source
gf	-191.36	kJ/mol	Joback Method
hf	-380.97	kJ/mol	Joback Method
hfus	19.45	kJ/mol	Joback Method
hvap	58.51	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	1.776		Crippen Method
mcvol	151.100	ml/mol	McGowan Method
pc	2986.06	kPa	Joback Method
rinpol	1478.00		NIST Webbook
tb	607.25	K	Joback Method
tc	824.77	K	Joback Method
tf	351.83	K	Joback Method
vc	0.579	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	364.06	J/mol×K	607.25	Joback Method
cpg	376.97	J/mol×K	643.50	Joback Method
cpg	389.08	J/mol×K	679.76	Joback Method
cpg	400.42	J/mol×K	716.01	Joback Method
cpg	410.99	J/mol×K	752.26	Joback Method
cpg	420.82	J/mol×K	788.52	Joback Method
cpg	429.92	J/mol×K	824.77	Joback Method
dvisc	0.0021334	Pa×s	351.83	Joback Method
dvisc	0.0011812	Pa×s	394.40	Joback Method

dvisc	0.0007338	Pa×s	436.97	Joback Method
dvisc	0.0004961	Pa×s	479.54	Joback Method
dvisc	0.0003575	Pa×s	522.11	Joback Method
dvisc	0.0002707	Pa×s	564.68	Joback Method
dvisc	0.0002131	Pa×s	607.25	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=R399509&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume