3-Butenoic acid, 4-phenyl-

Other names: Styrylacetic acid
4-Phenyl-3-butenoic acid
Inchi: InChI=1S/C10H10O2/c11-10(12)8-4-7-9-5-2-1-3-6-9/h1-7H,8H2,(H,11,12)/b7-4+
InchiKey: PSCXFXNEYIHJST-QPJJXVBHSA-N
Formula: C10H10O2
SMILES: O=C(O)CC=Cc1ccccc1
Mol. weight [g/mol]: 162.19
CAS: 2243-53-0

Physical Properties

Property code	Value	Unit	Source
gf	-39.79	kJ/mol	Joback Method
hf	-160.79	kJ/mol	Joback Method
hfus	21.59	kJ/mol	Joback Method
hvap	63.51	kJ/mol	Joback Method
log10ws	-2.23		Crippen Method
logp	2.174		Crippen Method
mcvol	131.140	ml/mol	McGowan Method
pc	3718.02	kPa	Joback Method
tb	605.09	K	Joback Method
tc	813.63	K	Joback Method
tf	360.15 ± 2.00	K	NIST Webbook
vc	0.492	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	306.84	J/mol×K	605.09	Joback Method
cpg	317.49	J/mol×K	639.85	Joback Method
cpg	327.42	J/mol×K	674.60	Joback Method
cpg	336.68	J/mol×K	709.36	Joback Method
cpg	345.31	J/mol×K	744.12	Joback Method
cpg	353.35	J/mol×K	778.87	Joback Method
cpg	360.85	J/mol×K	813.63	Joback Method

dvisc	0.0057762	Pa×s	334.55	Joback Method
dvisc	0.0018366	Pa×s	379.64	Joback Method
dvisc	0.0007448	Pa×s	424.73	Joback Method
dvisc	0.0003592	Pa×s	469.82	Joback Method
dvisc	0.0001968	Pa×s	514.91	Joback Method
dvisc	0.0001188	Pa×s	560.00	Joback Method
dvisc	0.0000773	Pa×s	605.09	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C2243530&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