2-Butenoic acid, isomer # 1

Inchi: InChI=1S/C4H6O2/c1-2-3-4(5)6/h2-3H,1H3,(H,5,6)/b3-2-
InchiKey: LDHQCZJRKDOVOX-IHWYPQMZSA-N
Formula: C4H6O2
SMILES: CC=CC(=O)O
Mol. weight [g/mol]: 86.09

Physical Properties

Property code	Value	Unit	Source
gf	-202.72	kJ/mol	Joback Method
hf	-273.48	kJ/mol	Joback Method
hfus	12.01	kJ/mol	Joback Method
hvap	47.88	kJ/mol	Joback Method
log10ws	-0.45		Crippen Method
logp	0.647		Crippen Method
mcvol	70.360	ml/mol	McGowan Method
pc	5138.68	kPa	Joback Method
ripol	1651.00		NIST Webbook
ripol	1651.00		NIST Webbook
tb	441.13	K	Joback Method
tc	623.44	K	Joback Method
tf	240.51	K	Joback Method
vc	0.265	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	129.47	J/mol×K	441.13	Joback Method
cpg	156.65	J/mol×K	593.05	Joback Method
cpg	151.79	J/mol×K	562.67	Joback Method
cpg	146.65	J/mol×K	532.28	Joback Method
cpg	141.22	J/mol×K	501.90	Joback Method
cpg	135.50	J/mol×K	471.51	Joback Method
cpg	161.26	J/mol×K	623.44	Joback Method
dvisc	0.0002256	Pa×s	441.13	Joback Method

dvisc	0.0003678	Pa×s	407.69	Joback Method
dvisc	0.0006544	Pa×s	374.26	Joback Method
dvisc	0.0013037	Pa×s	340.82	Joback Method
dvisc	0.0030171	Pa×s	307.38	Joback Method
dvisc	0.0085700	Pa×s	273.95	Joback Method
dvisc	0.0325411	Pa×s	240.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R518700&Units=SI
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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume