

(2E)-2-butenedioic acid

Inchi:	InChI=1S/C4H4O4/c5-3(6)1-2-4(7)8/h1-2H,(H,5,6)(H,7,8)/b2-1+
InchiKey:	VZCYOOQTPOCHFL-OWOJBTEDSA-N
Formula:	C4H4O4
SMILES:	O=C(O)C=CC(=O)O
Mol. weight [g/mol]:	116.07

Physical Properties

Property code	Value	Unit	Source
gf	-468.46	kJ/mol	Joback Method
hf	-538.29	kJ/mol	Joback Method
hfus	17.69	kJ/mol	Joback Method
hvap	71.31	kJ/mol	Joback Method
log10ws	0.45		Crippen Method
logp	-0.288		Crippen Method
mcvol	77.800	ml/mol	McGowan Method
pc	6503.64	kPa	Joback Method
tb	587.18	K	Joback Method
tc	769.82	K	Joback Method
tf	351.26	K	Joback Method
vc	0.289	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	168.01	J/molxK	587.18	Joback Method
cpg	172.46	J/molxK	617.62	Joback Method
cpg	176.64	J/molxK	648.06	Joback Method
cpg	180.57	J/molxK	678.50	Joback Method
cpg	184.27	J/molxK	708.94	Joback Method
cpg	187.74	J/molxK	739.38	Joback Method
cpg	191.01	J/molxK	769.82	Joback Method
dvisc	0.0094225	Paxs	351.26	Joback Method
dvisc	0.0025249	Paxs	390.58	Joback Method
dvisc	0.0008609	Paxs	429.90	Joback Method

dvisc	0.0003515	Paxs	469.22	Joback Method
dvisc	0.0001649	Paxs	508.54	Joback Method
dvisc	0.0000862	Paxs	547.86	Joback Method
dvisc	0.0000492	Paxs	587.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6001278&Units=SI
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

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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