1,3-Butadiene-1-carboxylic acid

Other names:	2,4-Pentadienoic acid
	«beta»-Vinylacrylic acid
	Butadiene-1-carboxylic acid
	«alpha»,«gamma»-Pentadienoic acid
	penta-2,4-dienoic acid
Inchi:	InChI=1S/C5H6O2/c1-2-3-4-5(6)7/h2-4H,1H2,(H,6,7)/b4-3+
InchiKey:	SDVVLIIVFBKBMG-ONEGZZNKSA-N
Formula:	C5H6O2
SMILES:	C=CC=CC(=O)O
Mol. weight [g/mol]:	98.10
CAS:	626-99-3

Physical Properties

Property code	Value	Unit	Source
gf	-106.46	kJ/mol	Joback Method
hf	-168.69	kJ/mol	Joback Method
hfus	13.31	kJ/mol	Joback Method
hvap	49.44	kJ/mol	Joback Method
log10ws	-0.72		Crippen Method
logp	0.813		Crippen Method
mcvol	80.150	ml/mol	McGowan Method
pc	4762.81	kPa	Joback Method
tb	460.69	K	Joback Method
tc	645.09	K	Joback Method
tf	250.02	K	Joback Method
vc	0.301	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	150.49	J/mol×K	460.69	Joback Method
cpg	157.04	J/mol×K	491.42	Joback Method
cpg	163.22	J/mol×K	522.16	Joback Method
cpg	169.04	J/mol×K	552.89	Joback Method

cpg	174.52	J/mol×K	583.62	Joback Method
cpg	179.69	J/mol×K	614.36	Joback Method
cpg	184.57	J/mol×K	645.09	Joback Method
dvisc	0.0258239	Pa×s	250.02	Joback Method
dvisc	0.0069735	Pa×s	285.13	Joback Method
dvisc	0.0025093	Pa×s	320.24	Joback Method
dvisc	0.0011050	Pa×s	355.36	Joback Method
dvisc	0.0005640	Pa×s	390.47	Joback Method
dvisc	0.0003216	Pa×s	425.58	Joback Method
dvisc	0.0001998	Pa×s	460.69	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=C626993&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