Butylmalonic acid

Other names:	Propanedioic acid, butyl-
	«alpha»-Carboxycaproic acid
	n-Butylmalonic acid
	Butylmalonate
	Malonic acid, butyl-
	1,1-Pentanedicarboxylic acid
	2-n-Butylmalonic acid
	2-Butylmalonate
	2-Butylmalonic acid
Inchi:	InChI=1S/C7H12O4/c1-2-3-4-5(6(8)9)7(10)11/h5H,2-4H2,1H3,(H,8,9)(H,10,11)
InchiKey:	MCRZWYDXIGCFKO-UHFFFAOYSA-N
Formula:	C7H12O4
SMILES:	CCCCC(C(=O)O)C(=O)O
Mol. weight [g/mol]:	160.17
CAS:	534-59-8

Physical Properties

Property code	Value	Unit	Source
chs	-3475.70	kJ/mol	NIST Webbook
gf	-525.86	kJ/mol	Joback Method
hf	-722.71	kJ/mol	Joback Method
hfus	21.74	kJ/mol	Joback Method
hsub	124.60 ± 2.30	kJ/mol	NIST Webbook
hvap	77.64	kJ/mol	Joback Method
log10ws	-0.71		Crippen Method
logp	0.962		Crippen Method
mcvol	124.370	ml/mol	McGowan Method
pc	4046.64	kPa	Joback Method
tb	651.22	K	Joback Method
tc	826.91	K	Joback Method
tf	375.15	K	Joback Method
vc	0.471	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.86	J/mol×K	651.22	Joback Method
cpg	360.95	J/mol×K	797.63	Joback Method
cpg	354.49	J/mol×K	768.35	Joback Method
cpg	347.66	J/mol×K	739.07	Joback Method
cpg	340.46	J/mol×K	709.78	Joback Method
cpg	332.86	J/mol×K	680.50	Joback Method
cpg	367.05	J/mol×K	826.91	Joback Method
dvisc	0.0000280	Pa×s	651.22	Joback Method
dvisc	0.0000498	Pa×s	605.21	Joback Method
dvisc	0.0000974	Pa×s	559.20	Joback Method
dvisc	0.0002150	Pa×s	513.19	Joback Method
dvisc	0.0005549	Pa×s	467.17	Joback Method
dvisc	0.0017611	Pa×s	421.16	Joback Method
dvisc	0.0074203	Pa×s	375.15	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=C534598&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs: Standard solid enthalpy of combustion
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
hsub: Enthalpy of sublimation 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