

Butanoic acid, 2-methyl-, (2S)-

Other names:	(S)-(+)-2-Methylbutyric acid Butanoic acid, 2-methyl-, (S)-
Inchi:	InChI=1S/C5H10O2/c1-3-4(2)5(6)7/h4H,3H2,1-2H3,(H,6,7)/t4-/m1/s1
InchiKey:	WLAMNBDJUVNPJU-SCSAIBSYSA-N
Formula:	C5H10O2
SMILES:	CCC(C)C(=O)O
Mol. weight [g/mol]:	102.13
CAS:	1730-91-2

Physical Properties

Property code	Value	Unit	Source
gf	-276.96	kJ/mol	Joback Method
hf	-416.62	kJ/mol	Joback Method
hfus	10.87	kJ/mol	Joback Method
hvap	49.76	kJ/mol	Joback Method
log10ws	-0.77		Crippen Method
logp	1.117		Crippen Method
mcvol	88.750	ml/mol	McGowan Method
pc	4244.08	kPa	Joback Method
tb	459.41	K	Joback Method
tc	635.76	K	Joback Method
tf	241.86	K	Joback Method
vc	0.335	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	183.94	J/mol×K	459.41	Joback Method
cpg	191.99	J/mol×K	488.80	Joback Method
cpg	199.72	J/mol×K	518.19	Joback Method
cpg	207.12	J/mol×K	547.58	Joback Method
cpg	214.20	J/mol×K	576.97	Joback Method
cpg	220.97	J/mol×K	606.37	Joback Method
cpg	227.44	J/mol×K	635.76	Joback Method

dvisc	0.0540168	Pa×s	241.86	Joback Method
dvisc	0.0120393	Pa×s	278.12	Joback Method
dvisc	0.0037936	Pa×s	314.38	Joback Method
dvisc	0.0015179	Pa×s	350.63	Joback Method
dvisc	0.0007211	Pa×s	386.89	Joback Method
dvisc	0.0003892	Pa×s	423.15	Joback Method
dvisc	0.0002315	Pa×s	459.41	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	351.20	K	2.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1730912&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

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
tbrp:	Boiling point at reduced pressure

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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