

Butanoic acid, 2-ethyl-2-methyl-

Other names:	2-Ethyl-2-methylbutanoic acid 2-Methyl-2-ethylbutanoic acid 2-ethyl-2-methylbutyric acid Butyric acid, 2-ethyl-2-methyl-
Inchi:	InChI=1S/C7H14O2/c1-4-7(3,5-2)6(8)9/h4-5H2,1-3H3,(H,8,9)
InchiKey:	LHJPKLWGGMAUAN-UHFFFAOYSA-N
Formula:	C7H14O2
SMILES:	CCC(C)(CC)C(=O)O
Mol. weight [g/mol]:	130.18
CAS:	19889-37-3

Physical Properties

Property code	Value	Unit	Source
gf	-254.84	kJ/mol	Joback Method
hf	-461.37	kJ/mol	Joback Method
hfus	12.16	kJ/mol	Joback Method
hvap	53.31	kJ/mol	Joback Method
log10ws	-1.61		Crippen Method
logp	1.897		Crippen Method
mcvol	116.930	ml/mol	McGowan Method
pc	3395.98	kPa	Joback Method
tb	502.38	K	Joback Method
tc	682.23	K	Joback Method
tf	281.82	K	Joback Method
vc	0.442	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.88	J/molxK	502.38	Joback Method
cpg	317.16	J/molxK	652.26	Joback Method
cpg	308.52	J/molxK	622.28	Joback Method
cpg	299.40	J/molxK	592.31	Joback Method
cpg	289.76	J/molxK	562.33	Joback Method

cpg	279.60	J/mol×K	532.36	Joback Method
cpg	325.33	J/mol×K	682.23	Joback Method
dvisc	0.0001723	Paxs	502.38	Joback Method
dvisc	0.0002838	Paxs	465.62	Joback Method
dvisc	0.0005092	Paxs	428.86	Joback Method
dvisc	0.0010196	Paxs	392.10	Joback Method
dvisc	0.0023568	Paxs	355.34	Joback Method
dvisc	0.0066100	Paxs	318.58	Joback Method
dvisc	0.0242619	Paxs	281.82	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.51007e+01
Coeff. B	-4.28329e+03
Coeff. C	-7.46320e+01
Temperature range (K), min.	363.79
Temperature range (K), max.	512.18

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=C19889373&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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