BUTANOIC ACID, 2,2-DIETHYL-

Inchi: InChI=1S/C8H16O2/c1-4-8(5-2,6-3)7(9)10/h4-6H2,1-3H3,(H,9,10)
InchiKey: GHXNRYVDXNZXID-UHFFFAOYSA-N
Formula: C8H16O2
SMILES: CCC(CC)(CC)C(=O)O
Mol. weight [g/mol]: 144.21

Physical Properties

Property code	Value	Unit	Source
af	0.6151		Cheméo Relay (1.0)
gf	-246.42	kJ/mol	Joback Method
hf	-560.17	kJ/mol	Cheméo Relay (1.0)
hfus	14.75	kJ/mol	Joback Method
hvap	72.93	kJ/mol	Cheméo Relay (1.0)
ie	9.82	eV	Cheméo Relay (1.0)
logp	2.287		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
pc	3045.68	kPa	Joback Method
tb	491.79	K	Cheméo Relay (1.0)
tc	680.73	K	Cheméo Relay (1.0)
tf	312.15 ± 2.00	K	NIST Webbook
vc	0.439	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.82	J/mol×K	525.26	Joback Method
cpg	324.40	J/mol×K	554.95	Joback Method
cpg	335.40	J/mol×K	584.64	Joback Method
cpg	345.83	J/mol×K	614.33	Joback Method
cpg	355.72	J/mol×K	644.02	Joback Method
cpg	365.10	J/mol×K	673.71	Joback Method
cpg	373.98	J/mol×K	703.40	Joback Method
dvisc	0.0196912	Pa×s	293.09	Joback Method
dvisc	0.0053599	Pa×s	331.79	Joback Method

dvisc	0.0019147	Pa×s	370.48	Joback Method
dvisc	0.0008310	Pa×s	409.18	Joback Method
dvisc	0.0004166	Pa×s	447.87	Joback Method
dvisc	0.0002331	Pa×s	486.56	Joback Method
dvisc	0.0001421	Pa×s	525.26	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C813581&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

af: Acentric Factor
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
ie: Ionization energy
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