

Butanoic acid, 2-ethyl-3,3-dimethyl, ethyl ester

Inchi:	InChI=1S/C10H20O2/c1-6-8(10(3,4)5)9(11)12-7-2/h8H,6-7H2,1-5H3
InchiKey:	JNJKJGSJFOZIA-UHFFFAOYSA-N
Formula:	C10H20O2
SMILES:	CCOC(=O)C(CC)C(C)(C)C
Mol. weight [g/mol]:	172.26

Physical Properties

Property code	Value	Unit	Source
gf	-200.20	kJ/mol	Joback Method
hf	-508.56	kJ/mol	Joback Method
hfus	13.51	kJ/mol	Joback Method
hvap	45.33	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	2.622		Crippen Method
mvol	159.200	ml/mol	McGowan Method
pc	2256.81	kPa	Joback Method
rinpol	1033.00		NIST Webbook
rinpol	1033.00		NIST Webbook
tb	500.82	K	Joback Method
tc	686.98	K	Joback Method
tf	262.04	K	Joback Method
vc	0.603	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.17	J/molxK	500.82	Joback Method
cpg	386.77	J/molxK	531.85	Joback Method
cpg	401.63	J/molxK	562.87	Joback Method
cpg	415.78	J/molxK	593.90	Joback Method
cpg	429.24	J/molxK	624.93	Joback Method
cpg	442.02	J/molxK	655.96	Joback Method
cpg	454.15	J/molxK	686.98	Joback Method
dvisc	0.0064596	Paxs	262.04	Joback Method

dvisc	0.0024849	Paxs	301.84	Joback Method
dvisc	0.0011942	Paxs	341.63	Joback Method
dvisc	0.0006687	Paxs	381.43	Joback Method
dvisc	0.0004178	Paxs	421.23	Joback Method
dvisc	0.0002831	Paxs	461.02	Joback Method
dvisc	0.0002041	Paxs	500.82	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R108239&Units=SI

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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