ETHYL 3,3-DIMETHYLBUTYRATE

Other names:	Ethyl 3,3-dimethylbutyrate
	Ethyl tert-butylacetate
	Butanoic acid, 3,3-dimethyl-, ethyl ester
	Ethyl 3,3-dimethylbutanoate
Inchi:	InChI=1S/C8H16O2/c1-5-10-7(9)6-8(2,3)4/h5-6H2,1-4H3
InchiKey:	JWMNHAMYTBAUPI-UHFFFAOYSA-N
Formula:	C8H16O2
SMILES:	CCOC(=O)CC(C)(C)C
Mol. weight [g/mol]:	144.21

Physical Properties

Property code	Value	Unit	Source
af	0.4419		Cheméo Relay (1.0)
gf	-214.60	kJ/mol	Joback Method
hf	-553.81	kJ/mol	Cheméo Relay (1.0)
hfus	11.85	kJ/mol	Joback Method
hvap	44.45	kJ/mol	Cheméo Relay (1.0)
ie	9.46	eV	Cheméo Relay (1.0)
log10ws	-1.99		Cheméo Relay (1.0)
logp	1.986		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
pc	2709.85	kPa	Joback Method
rinpol	878.00		NIST Webbook
rinpol	878.00		NIST Webbook
tb	401.61	K	Cheméo Relay (1.0)
tc	596.83	K	Cheméo Relay (1.0)
tf	224.65	K	Cheméo Relay (1.0)
vc	0.478	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.32	J/mol×K	455.50	Joback Method
cpg	353.92	J/mol×K	641.54	Joback Method

cpg	343.41	J/mol×K	610.54	Joback Method
cpg	332.35	J/mol×K	579.53	Joback Method
cpg	320.73	J/mol×K	548.52	Joback Method
cpg	308.53	J/mol×K	517.51	Joback Method
cpg	295.73	J/mol×K	486.51	Joback Method
dvisc	0.0007301	Pa×s	355.00	Joback Method
dvisc	0.0002582	Pa×s	455.50	Joback Method
dvisc	0.0003456	Pa×s	422.00	Joback Method
dvisc	0.0004864	Pa×s	388.50	Joback Method
dvisc	0.0046923	Pa×s	254.50	Joback Method
dvisc	0.0011929	Pa×s	321.50	Joback Method
dvisc	0.0021847	Pa×s	288.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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=C5340783&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
log10ws:	Log10 of Water solubility in mol/l
logp:	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

Latest version available from:
https://www.chemeo.com/cid/36-911-0/ETHYL-3-3-DIMETHYLBUTYRATE.pdf
Generated by Cheméo on 2026-07-21 09:44:42.562807811 +0000 UTC m=+138178.404693223.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.