Propanoic acid, 1,1-dimethylpropyl ester

Other names: 1,1-dimethylpropyl propanoate
2-butanol, 2-methyl-, propanoate
tert-amyl propionate
Inchi: InChI=1S/C8H16O2/c1-5-7(9)10-8(3,4)6-2/h5-6H2,1-4H3
InchiKey: RHSLWHLBYFOBAF-UHFFFAOYSA-N
Formula: C8H16O2
SMILES: CCC(=O)OC(C)(C)CC
Mol. weight [g/mol]: 144.21

Physical Properties

Property code	Value	Unit	Source
gf	-214.60	kJ/mol	Joback Method
hf	-462.00	kJ/mol	Joback Method
hfus	11.85	kJ/mol	Joback Method
hvap	41.26	kJ/mol	Joback Method
log10ws	-2.15		Crippen Method
logp	2.128		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
pc	2709.85	kPa	Joback Method
rinpol	893.00		NIST Webbook
rinpol	847.00		NIST Webbook
rinpol	847.00		NIST Webbook
rinpol	887.00		NIST Webbook
rinpol	888.00		NIST Webbook
rinpol	873.00		NIST Webbook
ripol	1087.00		NIST Webbook
ripol	1089.00		NIST Webbook
ripol	1108.00		NIST Webbook
ripol	1108.00		NIST Webbook
tb	455.50	K	Joback Method
tc	641.54	K	Joback Method
tf	254.50	K	Joback Method
vc	0.496	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.92	J/mol×K	641.54	Joback Method
cpg	295.73	J/mol×K	486.51	Joback Method
cpg	308.53	J/mol×K	517.51	Joback Method
cpg	320.73	J/mol×K	548.52	Joback Method
cpg	332.35	J/mol×K	579.53	Joback Method
cpg	343.41	J/mol×K	610.54	Joback Method
cpg	282.32	J/mol×K	455.50	Joback Method
dvisc	0.0003456	Pa×s	422.00	Joback Method
dvisc	0.0004864	Pa×s	388.50	Joback Method
dvisc	0.0007301	Pa×s	355.00	Joback Method
dvisc	0.0011929	Pa×s	321.50	Joback Method
dvisc	0.0021847	Pa×s	288.00	Joback Method
dvisc	0.0002582	Pa×s	455.50	Joback Method
dvisc	0.0046923	Pa×s	254.50	Joback Method
pvap	0.27	kPa	286.00	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.41	kPa	292.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.50	kPa	295.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.60	kPa	298.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.72	kPa	301.20	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters

pvap	0.85	kPa	304.30	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	1.02	kPa	307.40	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	1.24	kPa	310.40	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.22	kPa	283.00	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.19	kPa	281.00	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.17	kPa	278.90	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.14	kPa	276.90	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.12	kPa	274.90	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters
pvap	0.11	kPa	273.90	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters

pvap	0.33	kPa	289.10	Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters

Sources

Transpiration method: Vapor pressures and enthalpies of vaporization of some low-boiling esters:	https://www.doi.org/10.1016/j.fluid.2008.02.001
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=R113612&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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