Propanoic acid, 1,2-dimethylpropyl ester

Inchi: InChI=1S/C8H16O2/c1-5-8(9)10-7(4)6(2)3/h6-7H,5H2,1-4H3
InchiKey: RYYMZRUXQWULCT-UHFFFAOYSA-N
Formula: C8H16O2
SMILES: CCC(=O)OC(C)C(C)C
Mol. weight [g/mol]: 144.21

Physical Properties

Property code	Value	Unit	Source
gf	-222.32	kJ/mol	Joback Method
hf	-463.81	kJ/mol	Joback Method
hfus	12.22	kJ/mol	Joback Method
hvap	41.78	kJ/mol	Joback Method
log10ws	-1.90		Crippen Method
logp	1.984		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
pc	2701.41	kPa	Joback Method
rinpol	901.00		NIST Webbook
rinpol	893.00		NIST Webbook
rinpol	908.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	910.00		NIST Webbook
rinpol	913.00		NIST Webbook
ripol	1130.00		NIST Webbook
ripol	1130.00		NIST Webbook
ripol	1125.00		NIST Webbook
ripol	1121.00		NIST Webbook
tb	457.85	K	Joback Method
tc	640.65	K	Joback Method
tf	222.08	K	Joback Method
vc	0.495	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	279.95	J/mol×K	457.85	Joback Method
cpg	292.89	J/mol×K	488.32	Joback Method
cpg	305.35	J/mol×K	518.78	Joback Method
cpg	317.32	J/mol×K	549.25	Joback Method
cpg	328.83	J/mol×K	579.72	Joback Method
cpg	339.86	J/mol×K	610.19	Joback Method
cpg	350.42	J/mol×K	640.65	Joback Method
dvisc	0.0076048	Pa×s	222.08	Joback Method
dvisc	0.0027406	Pa×s	261.38	Joback Method
dvisc	0.0012896	Pa×s	300.67	Joback Method
dvisc	0.0007223	Pa×s	339.97	Joback Method
dvisc	0.0004562	Pa×s	379.26	Joback Method
dvisc	0.0003141	Pa×s	418.56	Joback Method
dvisc	0.0002306	Pa×s	457.85	Joback Method

Sources

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=R113627&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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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