

2-Methylpropanoic acid, 2,2-dimethyl-1-(2-hydroxy-1-methylethyl)propyl

Inchi:
ester

InChI=1S/C12H24O3/c1-8(2)11(14)15-10(9(3)7-13)12(4,5)6/h8-10,13H,7H2,1-6H3

InchiKey:

YXISVHDWGVMPGJ-UHFFFAOYSA-N

Formula:

C12H24O3

SMILES:

CC(C)C(=O)OC(C(C)CO)C(C)(C)C

Mol. weight [g/mol]:

216.32

Physical Properties

Property code	Value	Unit	Source
gf	-325.06	kJ/mol	Joback Method
hf	-712.63	kJ/mol	Joback Method
hfus	15.73	kJ/mol	Joback Method
hvap	65.68	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	2.229		Crippen Method
mcvol	193.250	ml/mol	McGowan Method
pc	2086.93	kPa	Joback Method
rinpol	1365.00		NIST Webbook
rinpol	1350.70		NIST Webbook
rinpol	1365.00		NIST Webbook
tb	637.88	K	Joback Method
tc	818.75	K	Joback Method
tf	315.40	K	Joback Method
vc	0.722	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	534.41	J/molxK	637.88	Joback Method
cpg	549.20	J/molxK	668.02	Joback Method
cpg	563.25	J/molxK	698.17	Joback Method
cpg	576.56	J/molxK	728.31	Joback Method
cpg	589.17	J/molxK	758.46	Joback Method
cpg	601.10	J/molxK	788.60	Joback Method
cpg	612.37	J/molxK	818.75	Joback Method

dvisc	0.0191716	Paxs	315.40	Joback Method
dvisc	0.0031940	Paxs	369.15	Joback Method
dvisc	0.0008392	Paxs	422.89	Joback Method
dvisc	0.0002981	Paxs	476.64	Joback Method
dvisc	0.0001306	Paxs	530.39	Joback Method
dvisc	0.0000666	Paxs	584.13	Joback Method
dvisc	0.0000380	Paxs	637.88	Joback Method

Sources

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=R398373&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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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