

(1-Methylpropyl)succinic acid, methyl ester

Inchi:	InChI=1S/C10H18O4/c1-5-7(2)8(10(12)14-4)6-9(11)13-3/h7-8H,5-6H2,1-4H3
InchiKey:	FDOGLQAJSDOFND-UHFFFAOYSA-N
Formula:	C10H18O4
SMILES:	CCC(C)C(CC(=O)OC)C(=O)OC
Mol. weight [g/mol]:	202.25

Physical Properties

Property code	Value	Unit	Source
gf	-439.40	kJ/mol	Joback Method
hf	-749.89	kJ/mol	Joback Method
hfus	20.18	kJ/mol	Joback Method
hvap	55.39	kJ/mol	Joback Method
log10ws	-1.25		Crippen Method
logp	1.385		Crippen Method
mcvol	166.640	ml/mol	McGowan Method
pc	2333.78	kPa	Joback Method
rinpol	1306.00		NIST Webbook
rinpol	1306.00		NIST Webbook
rinpol	1309.00		NIST Webbook
tb	579.90	K	Joback Method
tc	766.72	K	Joback Method
tf	316.78	K	Joback Method
vc	0.631	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	416.45	J/molxK	579.90	Joback Method
cpg	430.24	J/molxK	611.04	Joback Method
cpg	443.43	J/molxK	642.17	Joback Method
cpg	456.03	J/molxK	673.31	Joback Method
cpg	468.03	J/molxK	704.45	Joback Method
cpg	479.43	J/molxK	735.58	Joback Method
cpg	490.22	J/molxK	766.72	Joback Method

dvisc	0.0031886	Paxs	316.78	Joback Method
dvisc	0.0014437	Paxs	360.63	Joback Method
dvisc	0.0007762	Paxs	404.49	Joback Method
dvisc	0.0004712	Paxs	448.34	Joback Method
dvisc	0.0003126	Paxs	492.19	Joback Method
dvisc	0.0002218	Paxs	536.05	Joback Method
dvisc	0.0001658	Paxs	579.90	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=R292483&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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