

(1-Methylpentyl)succinic acid, methyl ester

Inchi:	InChI=1S/C12H22O4/c1-5-6-7-9(2)10(12(14)16-4)8-11(13)15-3/h9-10H,5-8H2,1-4H3
InchiKey:	NYGNRXFWKLHQRU-UHFFFAOYSA-N
Formula:	C12H22O4
SMILES:	CCCCC(C)C(CC(=O)OC)C(=O)OC
Mol. weight [g/mol]:	230.30

Physical Properties

Property code	Value	Unit	Source
gf	-422.56	kJ/mol	Joback Method
hf	-791.17	kJ/mol	Joback Method
hfus	25.36	kJ/mol	Joback Method
hvap	59.84	kJ/mol	Joback Method
log10ws	-2.09		Crippen Method
logp	2.165		Crippen Method
mcvol	194.820	ml/mol	McGowan Method
pc	1954.41	kPa	Joback Method
rinpol	1478.00		NIST Webbook
rinpol	1475.00		NIST Webbook
tb	625.66	K	Joback Method
tc	808.87	K	Joback Method
tf	339.32	K	Joback Method
vc	0.744	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	516.81	J/molxK	625.66	Joback Method
cpg	531.92	J/molxK	656.19	Joback Method
cpg	546.34	J/molxK	686.73	Joback Method
cpg	560.07	J/molxK	717.26	Joback Method
cpg	573.11	J/molxK	747.80	Joback Method
cpg	585.47	J/molxK	778.33	Joback Method
cpg	597.13	J/molxK	808.87	Joback Method
dvisc	0.0027555	Paxs	339.32	Joback Method

dvisc	0.0012154	Paxs	387.04	Joback Method
dvisc	0.0006416	Paxs	434.77	Joback Method
dvisc	0.0003843	Paxs	482.49	Joback Method
dvisc	0.0002525	Paxs	530.21	Joback Method
dvisc	0.0001778	Paxs	577.94	Joback Method
dvisc	0.0001321	Paxs	625.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R292478&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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