

3-Methyl-hept-2-enedioic acid dimethyl ester, E

Inchi:	InChI=1S/C9H14O4/c1-12-8(10)6-4-3-5-7-9(11)13-2/h4,6H,3,5,7H2,1-2H3/b6-4+
InchiKey:	PJYDYWXINWVDFD-GQCTYLIASA-N
Formula:	C9H14O4
SMILES:	COC(=O)C=CCCC(=O)OC
Mol. weight [g/mol]:	186.21

Physical Properties

Property code	Value	Unit	Source
gf	-362.72	kJ/mol	Joback Method
hf	-601.47	kJ/mol	Joback Method
hfus	24.84	kJ/mol	Joback Method
hvap	53.90	kJ/mol	Joback Method
log10ws	-1.17		Crippen Method
logp	1.059		Crippen Method
mcvol	148.250	ml/mol	McGowan Method
pc	2662.52	kPa	Joback Method
rinsol	1420.00		NIST Webbook
tb	562.06	K	Joback Method
tc	751.36	K	Joback Method
tf	330.43	K	Joback Method
vc	0.568	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.78	J/molxK	562.06	Joback Method
cpg	360.67	J/molxK	593.61	Joback Method
cpg	372.03	J/molxK	625.16	Joback Method
cpg	382.87	J/molxK	656.71	Joback Method
cpg	393.20	J/molxK	688.26	Joback Method
cpg	403.01	J/molxK	719.81	Joback Method
cpg	412.32	J/molxK	751.36	Joback Method
dvisc	0.0018275	Paxs	330.43	Joback Method
dvisc	0.0010108	Paxs	369.04	Joback Method

dvisc	0.0006254	Paxs	407.64	Joback Method
dvisc	0.0004205	Paxs	446.25	Joback Method
dvisc	0.0003012	Paxs	484.85	Joback Method
dvisc	0.0002266	Paxs	523.45	Joback Method
dvisc	0.0001773	Paxs	562.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R249300&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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