

Pentanedioic acid, 2,4-dimethyl-, dimethyl ester

Inchi:	InChI=1S/C9H16O4/c1-6(8(10)12-3)5-7(2)9(11)13-4/h6-7H,5H2,1-4H3
InchiKey:	LQLYZPTVIYLPB-UHFFFAOYSA-N
Formula:	C9H16O4
SMILES:	COC(=O)C(C)CC(C)C(=O)OC
Mol. weight [g/mol]:	188.22
CAS:	2121-68-8

Physical Properties

Property code	Value	Unit	Source
gf	-447.82	kJ/mol	Joback Method
hf	-729.25	kJ/mol	Joback Method
hfus	17.59	kJ/mol	Joback Method
hvap	53.16	kJ/mol	Joback Method
log10ws	-0.83		Crippen Method
logp	0.995		Crippen Method
mcvol	152.550	ml/mol	McGowan Method
pc	2566.29	kPa	Joback Method
tb	557.02	K	Joback Method
tc	745.99	K	Joback Method
tf	305.51	K	Joback Method
vc	0.576	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.76	J/molxK	557.02	Joback Method
cpg	381.74	J/molxK	588.51	Joback Method
cpg	394.19	J/molxK	620.01	Joback Method
cpg	406.09	J/molxK	651.50	Joback Method
cpg	417.44	J/molxK	683.00	Joback Method
cpg	428.24	J/molxK	714.49	Joback Method
cpg	438.48	J/molxK	745.99	Joback Method
dvisc	0.0033834	Paxs	305.51	Joback Method
dvisc	0.0015540	Paxs	347.43	Joback Method

dvisc	0.0008440	Paxs	389.35	Joback Method
dvisc	0.0005161	Paxs	431.26	Joback Method
dvisc	0.0003443	Paxs	473.18	Joback Method
dvisc	0.0002454	Paxs	515.10	Joback Method
dvisc	0.0001840	Paxs	557.02	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C2121688&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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