

Heptanedioic acid, 2,4-dimethyl-, dimethyl ester

Inchi:	InChI=1S/C11H20O4/c1-8(5-6-10(12)14-3)7-9(2)11(13)15-4/h8-9H,5-7H2,1-4H3
InchiKey:	TZCQHHKPFVJGT-UHFFFAOYSA-N
Formula:	C11H20O4
SMILES:	COC(=O)CCC(C)CC(C)C(=O)OC
Mol. weight [g/mol]:	216.27
CAS:	72719-04-1

Physical Properties

Property code	Value	Unit	Source
gf	-430.98	kJ/mol	Joback Method
hf	-770.53	kJ/mol	Joback Method
hfus	22.77	kJ/mol	Joback Method
hvap	57.62	kJ/mol	Joback Method
log10ws	-1.67		Crippen Method
logp	1.775		Crippen Method
mcvol	180.730	ml/mol	McGowan Method
pc	2131.49	kPa	Joback Method
rinpol	1380.00		NIST Webbook
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tb	602.78	K	Joback Method
tc	787.66	K	Joback Method
tf	328.05	K	Joback Method
vc	0.688	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	465.83	J/molxK	602.78	Joback Method
cpg	480.33	J/molxK	633.59	Joback Method
cpg	494.18	J/molxK	664.41	Joback Method
cpg	507.38	J/molxK	695.22	Joback Method
cpg	519.94	J/molxK	726.03	Joback Method
cpg	531.86	J/molxK	756.85	Joback Method
cpg	543.12	J/molxK	787.66	Joback Method

dvisc	0.0029767	Paxs	328.05	Joback Method
dvisc	0.0013297	Paxs	373.84	Joback Method
dvisc	0.0007082	Paxs	419.63	Joback Method
dvisc	0.0004269	Paxs	465.41	Joback Method
dvisc	0.0002818	Paxs	511.20	Joback Method
dvisc	0.0001992	Paxs	556.99	Joback Method
dvisc	0.0001484	Paxs	602.78	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=C72719041&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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