Heptanedioic acid, 4-methyl-, dimethyl ester

Other names: Dimethyl 4-methylheptanedioate
Inchi: InChI=1S/C10H18O4/c1-8(4-6-9(11)13-2)5-7-10(12)14-3/h8H,4-7H2,1-3H3
InchiKey: YBRNYBYNRKCRCW-UHFFFAOYSA-N
Formula: C10H18O4
SMILES: COC(=O)CCC(C)CCC(=O)OC
Mol. weight [g/mol]: 202.25
CAS: 4751-49-9

Physical Properties

Property code	Value	Unit	Source
gf	-436.96	kJ/mol	Joback Method
hf	-744.61	kJ/mol	Joback Method
hfus	23.71	kJ/mol	Joback Method
hvap	55.78	kJ/mol	Joback Method
log10ws	-1.49		Crippen Method
logp	1.529		Crippen Method
mcvol	166.640	ml/mol	McGowan Method
pc	2315.84	kPa	Joback Method
rinpol	1458.00		NIST Webbook
tb	580.34	K	Joback Method
tc	763.73	K	Joback Method
tf	331.78	K	Joback Method
vc	0.637	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	416.07	J/mol×K	580.34	Joback Method
cpg	477.83	J/mol×K	733.16	Joback Method
cpg	466.62	J/mol×K	702.60	Joback Method
cpg	454.83	J/mol×K	672.03	Joback Method
cpg	442.48	J/mol×K	641.47	Joback Method
cpg	429.55	J/mol×K	610.90	Joback Method
cpg	488.46	J/mol×K	763.73	Joback Method

dvisc	0.0001771	Pa×s	580.34	Joback Method
dvisc	0.0002316	Pa×s	538.91	Joback Method
dvisc	0.0003168	Pa×s	497.49	Joback Method
dvisc	0.0004587	Pa×s	456.06	Joback Method
dvisc	0.0007150	Pa×s	414.63	Joback Method
dvisc	0.0012300	Pa×s	373.21	Joback Method
dvisc	0.0024229	Pa×s	331.78	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=C4751499&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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