

Heptanedioic acid, 3-methyl-, dimethyl ester

Other names:	Dimethyl 3-methylheptane-1,7-dioate
Inchi:	InChI=1S/C10H18O4/c1-8(7-10(12)14-3)5-4-6-9(11)13-2/h8H,4-7H2,1-3H3
InchiKey:	HJRDWNWLAOQATD-UHFFFAOYSA-N
Formula:	C10H18O4
SMILES:	COC(=O)CCCC(C)CC(=O)OC
Mol. weight [g/mol]:	202.25
CAS:	54576-14-6

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	1351.00		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/molxK	580.34	Joback Method
cpg	429.55	J/molxK	610.90	Joback Method
cpg	442.48	J/molxK	641.47	Joback Method
cpg	454.83	J/molxK	672.03	Joback Method
cpg	466.62	J/molxK	702.60	Joback Method
cpg	477.83	J/molxK	733.16	Joback Method
cpg	488.46	J/molxK	763.73	Joback Method

dvisc	0.0024229	Paxs	331.78	Joback Method
dvisc	0.0012300	Paxs	373.21	Joback Method
dvisc	0.0007150	Paxs	414.63	Joback Method
dvisc	0.0004587	Paxs	456.06	Joback Method
dvisc	0.0003168	Paxs	497.49	Joback Method
dvisc	0.0002316	Paxs	538.91	Joback Method
dvisc	0.0001771	Paxs	580.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54576146&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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