Heptanedioic acid, dimethyl ester

Other names:	Dimethyl ester of heptanedioic acid
	Heptanedioic acid, methyl ester
	dimethyl 1,7-heptanedioate
	dimethyl heptanedioate
	dimethyl pimelate
	pimelic acid, dimethyl ester
Inchi:	InChI=1S/C9H16O4/c1-12-8(10)6-4-3-5-7-9(11)13-2/h3-7H2,1-2H3
InchiKey:	SHWINQXIGSEZAP-UHFFFAOYSA-N
Formula:	C9H16O4
SMILES:	COC(=O)CCCCCC(=O)OC
Mol. weight [g/mol]:	188.22
CAS:	1732-08-7

Physical Properties

Property code	Value	Unit	Source
chs	-4920.40	kJ/mol	NIST Webbook
gf	-442.94	kJ/mol	Joback Method
hf	-718.69	kJ/mol	Joback Method
hfus	24.64	kJ/mol	Joback Method
hvap	73.50 ± 0.30	kJ/mol	NIST Webbook
log10ws	-1.31		Crippen Method
logp	1.283		Crippen Method
mcvol	152.550	ml/mol	McGowan Method
pc	2370.00	kPa	Vapor Pressures, Enthalpies of Vaporization, and Critical Parameters of a Series of Linear Aliphatic Dimethyl Esters of Dicarboxylic Acids
rinpol	1307.00		NIST Webbook
rinpol	1345.00		NIST Webbook
rinpol	1313.00		NIST Webbook
rinpol	1344.70		NIST Webbook
rinpol	1307.00		NIST Webbook
rinpol	1309.00		NIST Webbook
rinpol	1309.00		NIST Webbook
rinpol	1313.00		NIST Webbook
rinpol	229.76		NIST Webbook

rinpol	1308.00		NIST Webbook
rinpol	229.76		NIST Webbook
rinpol	1313.00		NIST Webbook
rinpol	1308.00		NIST Webbook
rinpol	1310.00		NIST Webbook
rinpol	1345.00		NIST Webbook
rinpol	1346.00		NIST Webbook
rinpol	1346.00		NIST Webbook
rinpol	1308.00		NIST Webbook
rinpol	1344.70		NIST Webbook
ripol	1908.00		NIST Webbook
ripol	1908.00		NIST Webbook
ripol	1874.00		NIST Webbook
ripol	1874.00		NIST Webbook
ripol	1909.00		NIST Webbook
tb	557.90	K	Joback Method
tc	739.72	K	Joback Method
tf	255.30 ± 0.60	K	NIST Webbook
vc	0.588	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.05	J/mol×K	557.90	Joback Method
cpg	380.43	J/mol×K	588.20	Joback Method
cpg	392.33	J/mol×K	618.51	Joback Method
cpg	403.74	J/mol×K	648.81	Joback Method
cpg	414.66	J/mol×K	679.11	Joback Method
cpg	425.08	J/mol×K	709.42	Joback Method
cpg	435.00	J/mol×K	739.72	Joback Method
dvisc	0.0019834	Pa×s	335.51	Joback Method
dvisc	0.0011310	Pa×s	372.57	Joback Method
dvisc	0.0007139	Pa×s	409.64	Joback Method
dvisc	0.0004864	Pa×s	446.70	Joback Method
dvisc	0.0003515	Pa×s	483.77	Joback Method
dvisc	0.0002660	Pa×s	520.84	Joback Method
dvisc	0.0002089	Pa×s	557.90	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	394.70	K	1.50	NIST Webbook
tbrp	407.00 ± 1.00	K	2.40	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapor Pressures, Enthalpies of Vaporization, and Critical Parameters of a Series of Linear Aliphatic Dimethyl Esters of Dicarboxylic Acids:	https://www.doi.org/10.1021/je0602418
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=C1732087&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs:	Standard solid enthalpy of combustion
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume