

Pentanedioic acid, ethyl methyl ester

Other names:	Ethyl methyl diester of pentanedioic acid Methyl ethyll glutarate Glutaric acid, ethyl methyl ester Ethyl methyl glutarate
Inchi:	InChI=1S/C8H14O4/c1-3-12-8(10)6-4-5-7(9)11-2/h3-6H2,1-2H3
InchiKey:	YHRUNAIXGSNSTP-UHFFFAOYSA-N
Formula:	C8H14O4
SMILES:	CCOC(=O)CCCC(=O)OC
Mol. weight [g/mol]:	174.19
CAS:	51503-30-1

Physical Properties

Property code	Value	Unit	Source
gf	-451.36	kJ/mol	Joback Method
hf	-698.05	kJ/mol	Joback Method
hfus	22.05	kJ/mol	Joback Method
hvap	51.71	kJ/mol	Joback Method
log10ws	-0.90		Crippen Method
logp	0.893		Crippen Method
mcvol	138.460	ml/mol	McGowan Method
pc	2787.66	kPa	Joback Method
rinpol	1233.00		NIST Webbook
tb	535.02	K	Joback Method
tc	718.73	K	Joback Method
tf	324.24	K	Joback Method
vc	0.531	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.22	J/mol×K	535.02	Joback Method
cpg	333.68	J/mol×K	565.64	Joback Method
cpg	344.72	J/mol×K	596.26	Joback Method
cpg	355.33	J/mol×K	626.88	Joback Method

cpg	365.50	J/molxK	657.50	Joback Method
cpg	375.23	J/molxK	688.12	Joback Method
cpg	384.50	J/molxK	718.73	Joback Method
dvisc	0.0020386	Paxs	324.24	Joback Method
dvisc	0.0011847	Paxs	359.37	Joback Method
dvisc	0.0007583	Paxs	394.50	Joback Method
dvisc	0.0005222	Paxs	429.63	Joback Method
dvisc	0.0003804	Paxs	464.76	Joback Method
dvisc	0.0002898	Paxs	499.89	Joback Method
dvisc	0.0002287	Paxs	535.02	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=C51503301&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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