

Pentanedioic acid, 2-methylene-, dimethyl ester

Other names:	Glutaric acid, 2-methylene-, dimethyl ester Dimethyl 2-methyleneglutarate Dimethyl 2-methylenepentanedioate Methyl methyleneglutarate 1-Butene-2,4-dicarboxylic acid dimethyl ester 2-Methyleneglutaric acid, dimethyl ester 2,4-bis-(Methoxycarbonyl)-1-butene
Inchi:	InChI=1S/C8H12O4/c1-6(8(10)12-3)4-5-7(9)11-2/h1,4-5H2,2-3H3
InchiKey:	URLYMBMJTPDVEP-UHFFFAOYSA-N
Formula:	C8H12O4
SMILES:	C=C(CCC(=O)OC)C(=O)OC
Mol. weight [g/mol]:	172.18
CAS:	5621-44-3

Physical Properties

Property code	Value	Unit	Source
gf	-372.07	kJ/mol	Joback Method
hf	-582.41	kJ/mol	Joback Method
hfus	19.46	kJ/mol	Joback Method
hvap	51.12	kJ/mol	Joback Method
log10ws	-0.75		Crippen Method
logp	0.669		Crippen Method
mcvol	134.160	ml/mol	McGowan Method
pc	2931.34	kPa	Joback Method
rinpol	1180.00		NIST Webbook
rinpol	1180.00		NIST Webbook
tb	531.58	K	Joback Method
tc	722.05	K	Joback Method
tf	308.52	K	Joback Method
vc	0.513	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	303.30	J/mol×K	531.58	Joback Method
cpg	314.26	J/mol×K	563.33	Joback Method
cpg	324.78	J/mol×K	595.07	Joback Method
cpg	334.86	J/mol×K	626.82	Joback Method
cpg	344.48	J/mol×K	658.56	Joback Method
cpg	353.66	J/mol×K	690.31	Joback Method
cpg	362.37	J/mol×K	722.05	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C5621443&Units=SI

Legend

cpg:	Ideal gas heat capacity
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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