Diethyl glutaconate

Other names:	2-Pentenedioic acid, diethyl ester
	Glutaconic acid, diethyl ester
	Diethyl 2-pentenedioate
	diethyl pent-2-enedioate
Inchi:	InChI=1S/C9H14O4/c1-3-12-8(10)6-5-7-9(11)13-4-2/h5-6H,3-4,7H2,1-2H3/b6-5+
InchiKey:	JHCKGVJZNIWNJK-AATRIKPKSA-N
Formula:	C9H14O4
SMILES:	CCOC(=O)C=CCC(=O)OCC
Mol. weight [g/mol]:	186.21
CAS:	2049-67-4

Physical Properties

Property code	Value	Unit	Source
gf	-362.72	kJ/mol	Joback Method
hf	-601.47	kJ/mol	Joback Method
hfus	24.84	kJ/mol	Joback Method
hvap	53.90	kJ/mol	Joback Method
log10ws	-1.17		Crippen Method
logp	1.059		Crippen Method
mcvol	148.250	ml/mol	McGowan Method
pc	2662.52	kPa	Joback Method
tb	510.20	K	NIST Webbook
tc	751.36	K	Joback Method
tf	330.43	K	Joback Method
vc	0.568	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.78	J/mol×K	562.06	Joback Method
cpg	360.67	J/mol×K	593.61	Joback Method
cpg	372.03	J/mol×K	625.16	Joback Method
cpg	382.87	J/mol×K	656.71	Joback Method
cpg	393.20	J/mol×K	688.26	Joback Method

cpg	403.01	J/mol×K	719.81	Joback Method
cpg	412.32	J/mol×K	751.36	Joback Method
dvisc	0.0018275	Pa×s	330.43	Joback Method
dvisc	0.0010108	Pa×s	369.04	Joback Method
dvisc	0.0006254	Pa×s	407.64	Joback Method
dvisc	0.0004205	Pa×s	446.25	Joback Method
dvisc	0.0003012	Pa×s	484.85	Joback Method
dvisc	0.0002266	Pa×s	523.45	Joback Method
dvisc	0.0001773	Pa×s	562.06	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2049674&Units=SI
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

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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