Itaconic acid diethyl ester

Other names:	Butanedioic acid, methylene-, diethyl ester
	Diethyl itaconate
	Ethyl itaconate
	Succinic acid, methylene-, diethyl ester
	Butanedioic acid, 2-methylene, diethyl ester
	Diethyl 2-methylenesuccinate
	Butanedioic acid, 2-methylene-, 1,4-diethyl ester
Inchi:	InChI=1S/C9H14O4/c1-4-12-8(10)6-7(3)9(11)13-5-2/h3-6H2,1-2H3
InchiKey:	ZEFVHSWKYCYFFL-UHFFFAOYSA-N
Formula:	C9H14O4
SMILES:	C=C(CC(=O)OCC)C(=O)OCC
Mol. weight [g/mol]:	186.21
CAS:	2409-52-1

Physical Properties

Property code	Value	Unit	Source
gf	-363.65	kJ/mol	Joback Method
hf	-603.05	kJ/mol	Joback Method
hfus	22.05	kJ/mol	Joback Method
hvap	53.35	kJ/mol	Joback Method
log10ws	-1.17		Crippen Method
logp	1.059		Crippen Method
mcvol	148.250	ml/mol	McGowan Method
pc	2648.83	kPa	Joback Method
rinpol	1232.00		NIST Webbook
tb	554.46	K	Joback Method
tc	742.67	K	Joback Method
tf	319.79	K	Joback Method
vc	0.570	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.31	J/mol×K	554.46	Joback Method

cpg	360.23	J/mol×K	585.83	Joback Method
cpg	371.65	J/mol×K	617.20	Joback Method
cpg	382.57	J/mol×K	648.56	Joback Method
cpg	392.98	J/mol×K	679.93	Joback Method
cpg	402.89	J/mol×K	711.30	Joback Method
cpg	412.29	J/mol×K	742.67	Joback Method
hvapt	51.00	kJ/mol	412.50	NIST Webbook

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=C2409521&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
hvapt:	Enthalpy of vaporization at a given temperature
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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