Diethyl ethylidenemalonate

Other names:	Propanedioic acid, ethylidene-, diethyl ester
Inchi:	InChI=1S/C9H14O4/c1-4-7(8(10)12-5-2)9(11)13-6-3/h4H,5-6H2,1-3H3
InchiKey:	LBBAWVLUOZVYCC-UHFFFAOYSA-N
Formula:	C9H14O4
SMILES:	CC=C(C(=O)OCC)C(=O)OCC
Mol. weight [g/mol]:	186.21
CAS:	1462-12-0

Physical Properties

Property code	Value	Unit	Source
gf	-371.27	kJ/mol	Joback Method
hf	-611.26	kJ/mol	Joback Method
hfus	23.53	kJ/mol	Joback Method
hvap	53.98	kJ/mol	Joback Method
log10ws	-1.17		Crippen Method
logp	1.059		Crippen Method
mcvol	148.250	ml/mol	McGowan Method
pc	2676.31	kPa	Joback Method
tb	561.94	K	Joback Method
tc	754.41	K	Joback Method
tf	316.47	K	Joback Method
vc	0.569	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.59	J/mol×K	561.94	Joback Method
cpg	360.64	J/mol×K	594.02	Joback Method
cpg	372.16	J/mol×K	626.10	Joback Method
cpg	383.14	J/mol×K	658.17	Joback Method
cpg	393.58	J/mol×K	690.25	Joback Method
cpg	403.50	J/mol×K	722.33	Joback Method
cpg	412.90	J/mol×K	754.41	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	389.70	K	2.30	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1462120&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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