

Propanedioic acid, ethylmethyl-, diethyl ester

Other names:	diethyl ethylmethylmalonate
Inchi:	InChI=1S/C10H18O4/c1-5-10(4,8(11)13-6-2)9(12)14-7-3/h5-7H2,1-4H3
InchiKey:	ODRGILDUWDVBJX-UHFFFAOYSA-N
Formula:	C10H18O4
SMILES:	CCOC(=O)C(C)(CC)C(=O)OCC
Mol. weight [g/mol]:	202.25
CAS:	2049-70-9

Physical Properties

Property code	Value	Unit	Source
gf	-431.68	kJ/mol	Joback Method
hf	-748.08	kJ/mol	Joback Method
hfus	19.82	kJ/mol	Joback Method
hvap	54.87	kJ/mol	Joback Method
log10ws	-1.49		Crippen Method
logp	1.529		Crippen Method
mcvol	166.640	ml/mol	McGowan Method
pc	2340.56	kPa	Joback Method
tb	577.55	K	Joback Method
tc	767.26	K	Joback Method
tf	349.20	K	Joback Method
vc	0.632	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.32	J/molxK	767.26	Joback Method
cpg	418.99	J/molxK	577.55	Joback Method
cpg	432.86	J/molxK	609.17	Joback Method
cpg	446.07	J/molxK	640.79	Joback Method
cpg	458.60	J/molxK	672.40	Joback Method
cpg	470.48	J/molxK	704.02	Joback Method
cpg	481.72	J/molxK	735.64	Joback Method
dvisc	0.0001715	Paxs	577.55	Joback Method

dvisc	0.0021400	Paxs	349.20	Joback Method
dvisc	0.0011428	Paxs	387.26	Joback Method
dvisc	0.0006828	Paxs	425.32	Joback Method
dvisc	0.0004439	Paxs	463.38	Joback Method
dvisc	0.0003081	Paxs	501.43	Joback Method
dvisc	0.0002252	Paxs	539.49	Joback Method
hvapt	53.20	kJ/mol	399.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C2049709&Units=SI

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

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