

Tartronic acid, diethyl ester, acetate

Other names:	diethyl acetoxy malonate
Inchi:	InChI=1S/C9H14O6/c1-4-13-8(11)7(15-6(3)10)9(12)14-5-2/h7H,4-5H2,1-3H3
InchiKey:	XZFLUEMBCUUTKI-UHFFFAOYSA-N
Formula:	C9H14O6
SMILES:	CCOC(=O)C(OC(C)=O)C(=O)OCC
Mol. weight [g/mol]:	218.20
CAS:	5468-23-5

Physical Properties

Property code	Value	Unit	Source
gf	-679.30	kJ/mol	Joback Method
hf	-968.77	kJ/mol	Joback Method
hfus	23.90	kJ/mol	Joback Method
hvap	62.71	kJ/mol	Joback Method
log10ws	-0.29		Crippen Method
logp	0.044		Crippen Method
mcvol	159.990	ml/mol	McGowan Method
pc	2668.02	kPa	Joback Method
tb	633.75	K	Joback Method
tc	825.52	K	Joback Method
tf	392.67	K	Joback Method
vc	0.606	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.69	J/mol×K	633.75	Joback Method
cpg	421.38	J/mol×K	665.71	Joback Method
cpg	432.51	J/mol×K	697.67	Joback Method
cpg	443.06	J/mol×K	729.63	Joback Method
cpg	453.02	J/mol×K	761.60	Joback Method
cpg	462.37	J/mol×K	793.56	Joback Method
cpg	471.09	J/mol×K	825.52	Joback Method
dvisc	0.0014534	Paxs	392.67	Joback Method

dvisc	0.0008437	Paxs	432.85	Joback Method
dvisc	0.0005372	Paxs	473.03	Joback Method
dvisc	0.0003671	Paxs	513.21	Joback Method
dvisc	0.0002651	Paxs	553.39	Joback Method
dvisc	0.0002001	Paxs	593.57	Joback Method
dvisc	0.0001565	Paxs	633.75	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5468235&Units=SI
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

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_cvol:	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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