

Racem-dimethoxysuccinic acid, dimethylester

Inchi:	InChI=1S/C8H14O6/c1-3-13-7(11)5(9)6(10)8(12)14-4-2/h5-6,9-10H,3-4H2,1-2H3
InchiKey:	YSAVZVORKRDODB-UHFFFAOYSA-N
Formula:	C8H14O6
SMILES:	CCOC(=O)C(O)C(O)C(=O)OCC
Mol. weight [g/mol]:	206.19
CAS:	57968-71-5

Physical Properties

Property code	Value	Unit	Source
gf	-729.88	kJ/mol	Joback Method
hf	-1013.07	kJ/mol	Joback Method
hfus	23.18	kJ/mol	Joback Method
hvap	84.30	kJ/mol	Joback Method
log10ws	0.35		Crippen Method
logp	-1.166		Crippen Method
mcvol	150.200	ml/mol	McGowan Method
pc	3484.76	kPa	Joback Method
tb	718.50	K	Joback Method
tc	897.05	K	Joback Method
tf	415.88	K	Joback Method
vc	0.557	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	467.22	J/mol×K	897.05	Joback Method
cpg	421.19	J/mol×K	718.50	Joback Method
cpg	430.10	J/mol×K	748.26	Joback Method
cpg	438.51	J/mol×K	778.02	Joback Method
cpg	446.44	J/mol×K	807.78	Joback Method
cpg	453.87	J/mol×K	837.54	Joback Method
cpg	460.80	J/mol×K	867.29	Joback Method
dvisc	0.0000099	Pa×s	718.50	Joback Method
dvisc	0.0021532	Pa×s	415.88	Joback Method

dvisc	0.0005404	Pa×s	466.32	Joback Method
dvisc	0.0001777	Pa×s	516.75	Joback Method
dvisc	0.0000712	Pa×s	567.19	Joback Method
dvisc	0.0000331	Pa×s	617.63	Joback Method
dvisc	0.0000173	Pa×s	668.06	Joback Method
hsubt	60.20 ± 0.80	kJ/mol	303.00	NIST Webbook

Sources

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=C57968715&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hsubt:	Enthalpy of sublimation at a given temperature
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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