

Butanedioic acid, 2,3-dihydroxy-, bis(1-methylethyl) ester, [S-(R*,R*)]-

Other names:	Diisopropyl d-tartrate diisopropyl [S-(R*,R*)]-tartrate (d) diisopropyl tartrate
Inchi:	InChI=1S/C10H18O6/c1-5(2)15-9(13)7(11)8(12)10(14)16-6(3)4/h5-8,11-12H,1-4H3/t7-,8-
InchiKey:	XEBCWEDRGPSHQH-HTQZYQBOSA-N
Formula:	C10H18O6
SMILES:	CC(C)OC(=O)C(O)C(O)C(=O)OC(C)C
Mol. weight [g/mol]:	234.25
CAS:	62961-64-2

Physical Properties

Property code	Value	Unit	Source
gf	-717.92	kJ/mol	Joback Method
hf	-1064.91	kJ/mol	Joback Method
hfus	21.31	kJ/mol	Joback Method
hvap	87.97	kJ/mol	Joback Method
log10ws	-0.71		Crippen Method
logp	-0.389		Crippen Method
mcvol	178.380	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
rinpol	1385.20		NIST Webbook
rinpol	1385.20		NIST Webbook
tb	763.38	K	Joback Method
tc	946.82	K	Joback Method
tf	408.42	K	Joback Method
vc	0.657	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	578.84	J/mol×K	946.82	Joback Method
cpg	571.68	J/mol×K	916.24	Joback Method
cpg	563.88	J/mol×K	885.67	Joback Method
cpg	555.45	J/mol×K	855.10	Joback Method

cpg	546.38	J/mol×K	824.53	Joback Method
cpg	536.68	J/mol×K	793.95	Joback Method
cpg	526.34	J/mol×K	763.38	Joback Method
dvisc	0.0030290	Pa×s	408.42	Joback Method
dvisc	0.0000053	Pa×s	763.38	Joback Method
dvisc	0.0000098	Pa×s	704.22	Joback Method
dvisc	0.0000202	Pa×s	645.06	Joback Method
dvisc	0.0000483	Pa×s	585.90	Joback Method
dvisc	0.0001408	Pa×s	526.74	Joback Method
dvisc	0.0005379	Pa×s	467.58	Joback Method
hvapt	65.70	kJ/mol	462.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C62961642&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
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
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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