

1,3-Butanediol diformate

Inchi:	InChI=1S/C6H10O4/c1-6(10-5-8)2-3-9-4-7/h4-6H,2-3H2,1H3
InchiKey:	AAEDMUBUSKPAOR-UHFFFAOYSA-N
Formula:	C6H10O4
SMILES:	CC(CCOC=O)OC=O
Mol. weight [g/mol]:	146.14

Physical Properties

Property code	Value	Unit	Source
gf	-411.84	kJ/mol	Joback Method
hf	-608.05	kJ/mol	Joback Method
hfus	14.73	kJ/mol	Joback Method
hvap	46.82	kJ/mol	Joback Method
log10ws	-0.17		Crippen Method
logp	0.111		Crippen Method
mcvol	110.280	ml/mol	McGowan Method
pc	3577.07	kPa	Joback Method
rinpol	903.00		NIST Webbook
rinpol	903.00		NIST Webbook
rinpol	918.00		NIST Webbook
tb	478.40	K	Joback Method
tc	660.86	K	Joback Method
tf	270.84	K	Joback Method
vc	0.435	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	240.12	J/molxK	478.40	Joback Method
cpg	249.06	J/molxK	508.81	Joback Method
cpg	257.71	J/molxK	539.22	Joback Method
cpg	266.08	J/molxK	569.63	Joback Method
cpg	274.14	J/molxK	600.04	Joback Method
cpg	281.90	J/molxK	630.45	Joback Method
cpg	289.33	J/molxK	660.86	Joback Method

dvisc	0.0035190	Paxs	270.84	Joback Method
dvisc	0.0018461	Paxs	305.43	Joback Method
dvisc	0.0011043	Paxs	340.03	Joback Method
dvisc	0.0007263	Paxs	374.62	Joback Method
dvisc	0.0005128	Paxs	409.21	Joback Method
dvisc	0.0003822	Paxs	443.81	Joback Method
dvisc	0.0002973	Paxs	478.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R142511&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

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
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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