

1,1-Ethanediol, diisobutyrate

Inchi:	InChI=1S/C10H18O4/c1-6(2)9(11)13-8(5)14-10(12)7(3)4/h6-8H,1-5H3
InchiKey:	KQSKJYCVBSFALB-UHFFFAOYSA-N
Formula:	C10H18O4
SMILES:	CC(OC(=O)C(C)C)OC(=O)C(C)C
Mol. weight [g/mol]:	202.25
CAS:	116346-31-7

Physical Properties

Property code	Value	Unit	Source
gf	-441.84	kJ/mol	Joback Method
hf	-755.17	kJ/mol	Joback Method
hfus	16.66	kJ/mol	Joback Method
hvap	55.00	kJ/mol	Joback Method
log10ws	-1.86		Crippen Method
logp	1.731		Crippen Method
mcvol	166.640	ml/mol	McGowan Method
pc	2351.92	kPa	Joback Method
tb	579.46	K	Joback Method
tc	769.85	K	Joback Method
tf	301.78	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	416.83	J/molxK	579.46	Joback Method
cpg	481.08	J/molxK	738.11	Joback Method
cpg	469.49	J/molxK	706.38	Joback Method
cpg	457.27	J/molxK	674.65	Joback Method
cpg	444.41	J/molxK	642.92	Joback Method
cpg	430.93	J/molxK	611.19	Joback Method
cpg	492.02	J/molxK	769.85	Joback Method
dvisc	0.0001552	Paxs	579.46	Joback Method
dvisc	0.0002126	Paxs	533.18	Joback Method

dvisc	0.0003093	Paxs	486.90	Joback Method
dvisc	0.0004867	Paxs	440.62	Joback Method
dvisc	0.0008520	Paxs	394.34	Joback Method
dvisc	0.0017309	Paxs	348.06	Joback Method
dvisc	0.0043702	Paxs	301.78	Joback Method

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=C116346317&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
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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