

Diisobutyl oxalate

Other names:	Oxalic acid, diisobutyl ester
Inchi:	InChI=1S/C10H18O4/c1-7(2)5-13-9(11)10(12)14-6-8(3)4/h7-8H,5-6H2,1-4H3
InchiKey:	GJRRTUSXQPXVES-UHFFFAOYSA-N
Formula:	C10H18O4
SMILES:	CC(C)COC(=O)C(=O)OCC(C)C
Mol. weight [g/mol]:	202.25
CAS:	2050-61-5

Physical Properties

Property code	Value	Unit	Source
gf	-439.40	kJ/mol	Joback Method
hf	-749.89	kJ/mol	Joback Method
hfus	20.18	kJ/mol	Joback Method
hvap	55.39	kJ/mol	Joback Method
log10ws	-1.25		Crippen Method
logp	1.385		Crippen Method
mcvol	166.640	ml/mol	McGowan Method
pc	2333.78	kPa	Joback Method
rinpol	1236.00		NIST Webbook
rinpol	1236.00		NIST Webbook
tb	579.90	K	Joback Method
tc	766.72	K	Joback Method
tf	316.78	K	Joback Method
vc	0.631	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	490.22	J/mol×K	766.72	Joback Method
cpg	416.45	J/mol×K	579.90	Joback Method
cpg	430.24	J/mol×K	611.04	Joback Method
cpg	443.43	J/mol×K	642.17	Joback Method
cpg	456.03	J/mol×K	673.31	Joback Method
cpg	468.03	J/mol×K	704.45	Joback Method

cpg	479.43	J/mol×K	735.58	Joback Method
dvisc	0.0001658	Pa×s	579.90	Joback Method
dvisc	0.0031886	Pa×s	316.78	Joback Method
dvisc	0.0014437	Pa×s	360.63	Joback Method
dvisc	0.0007762	Pa×s	404.49	Joback Method
dvisc	0.0004712	Pa×s	448.34	Joback Method
dvisc	0.0003126	Pa×s	492.19	Joback Method
dvisc	0.0002218	Pa×s	536.05	Joback Method
hvapt	55.50	kJ/mol	419.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2050615&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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