

1-propen-1,3-dicarbaldehyde

Inchi:	InChI=1S/C5H6O2/c6-4-2-1-3-5-7/h1-2,4-5H,3H2/b2-1+
InchiKey:	NEOPYIBVKJWHMN-OWOJBTEDSA-N
Formula:	C5H6O2
SMILES:	O=CC=CCC=O
Mol. weight [g/mol]:	98.10

Physical Properties

Property code	Value	Unit	Source
gf	-127.60	kJ/mol	Joback Method
hf	-200.47	kJ/mol	Joback Method
hfus	13.49	kJ/mol	Joback Method
hvap	40.12	kJ/mol	Joback Method
log10ws	-0.33		Crippen Method
logp	0.330		Crippen Method
mcvol	80.150	ml/mol	McGowan Method
pc	4456.32	kPa	Joback Method
ripol	1969.00		NIST Webbook
ripol	1969.00		NIST Webbook
tb	415.28	K	Joback Method
tc	605.57	K	Joback Method
tf	225.03	K	Joback Method
vc	0.330	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	144.63	J/molxK	415.28	Joback Method
cpg	151.76	J/molxK	447.00	Joback Method
cpg	158.49	J/molxK	478.71	Joback Method
cpg	164.85	J/molxK	510.43	Joback Method
cpg	170.85	J/molxK	542.14	Joback Method
cpg	176.50	J/molxK	573.86	Joback Method
cpg	181.84	J/molxK	605.57	Joback Method
dvisc	0.0035287	Paxs	225.03	Joback Method

dvisc	0.0018847	Paxs	256.74	Joback Method
dvisc	0.0011554	Paxs	288.45	Joback Method
dvisc	0.0007804	Paxs	320.15	Joback Method
dvisc	0.0005658	Paxs	351.86	Joback Method
dvisc	0.0004326	Paxs	383.57	Joback Method
dvisc	0.0003446	Paxs	415.28	Joback Method

Sources

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=R492821&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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