

trans,trans-Muconic acid

Other names:	Muconic acid (trans) trans,trans-1,3-Butadiene-1,4-dicarboxylic acid 2,4-Hexadienedioic acid, (E,E)- (E,E)-Muconic acid trans,trans-buta-1,3-diene-1,4-dicarboxylic acid
Inchi:	InChI=1S/C6H6O4/c7-5(8)3-1-2-4-6(9)10/h1-4H,(H,7,8)(H,9,10)/b3-1+,4-2+
InchiKey:	TXXHDPDFNKHHGW-ZPUQHVIOSA-N
Formula:	C6H6O4
SMILES:	O=C(O)C=CC=CC(=O)O
Mol. weight [g/mol]:	142.11
CAS:	3588-17-8

Physical Properties

Property code	Value	Unit	Source
gf	-371.40	kJ/mol	Joback Method
hf	-462.35	kJ/mol	Joback Method
hfus	23.07	kJ/mol	Joback Method
hvap	75.72	kJ/mol	Joback Method
log10ws	-0.24		Crippen Method
logp	0.268		Crippen Method
mcvol	101.680	ml/mol	McGowan Method
pc	5251.00	kPa	Joback Method
tb	593.20	K	NIST Webbook
tc	823.04	K	Joback Method
tf	558.15 ± 5.00	K	NIST Webbook
vc	0.382	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	233.19	J/mol×K	637.10	Joback Method
cpg	258.15	J/mol×K	792.05	Joback Method
cpg	253.74	J/mol×K	761.06	Joback Method
cpg	249.06	J/mol×K	730.07	Joback Method

cpg	244.10	J/molxK	699.08	Joback Method
cpg	238.82	J/molxK	668.09	Joback Method
cpg	262.33	J/molxK	823.04	Joback Method
dvisc	0.0000260	Paxs	637.10	Joback Method
dvisc	0.0000457	Paxs	592.37	Joback Method
dvisc	0.0000881	Paxs	547.64	Joback Method
dvisc	0.0001909	Paxs	502.91	Joback Method
dvisc	0.0004810	Paxs	458.18	Joback Method
dvisc	0.0014798	Paxs	413.45	Joback Method
dvisc	0.0059797	Paxs	368.72	Joback Method

Sources

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=C3588178&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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