3-Methylglutakonic acid dimethyl ester

Other names: 3-Methyl-pent-2-enedioic acid dimethyl ester, E
trans-2-Pentenedioate, 3-methyl, dimethyl ester
Inchi: InChI=1S/C8H12O4/c1-6(4-7(9)11-2)5-8(10)12-3/h4H,5H2,1-3H3/b6-4+
InchiKey: GBQBEQOEGMZCOH-GQCTYLIASA-N
Formula: C8H12O4
SMILES: COC(=O)C=C(C)CC(=O)OC
Mol. weight [g/mol]: 172.18

Physical Properties

Property code	Value	Unit	Source
gf	-379.69	kJ/mol	Joback Method
hf	-590.62	kJ/mol	Joback Method
hfus	20.94	kJ/mol	Joback Method
hvap	51.75	kJ/mol	Joback Method
log10ws	-0.75		Crippen Method
logp	0.669		Crippen Method
mcvol	134.160	ml/mol	McGowan Method
pc	2963.34	kPa	Joback Method
rinpol	1198.00		NIST Webbook
rinpol	1195.00		NIST Webbook
tb	539.06	K	Joback Method
tc	734.03	K	Joback Method
tf	305.20	K	Joback Method
vc	0.512	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.31	J/mol×K	539.06	Joback Method
cpg	314.42	J/mol×K	571.56	Joback Method
cpg	325.05	J/mol×K	604.05	Joback Method
cpg	335.20	J/mol×K	636.55	Joback Method
cpg	344.87	J/mol×K	669.04	Joback Method
cpg	354.06	J/mol×K	701.54	Joback Method

cpg	362.77	J/mol×K	734.03	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U222064&Units=SI

Legend

cpg:	Ideal gas heat capacity
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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