

Glutaric acid, di(hexa-1,5-dien-3-yl) ester

Inchi:	InChI=1S/C17H24O4/c1-5-10-14(7-3)20-16(18)12-9-13-17(19)21-15(8-4)11-6-2/h5-8,14-
InchiKey:	QLLHSTAIPKHPMR-UHFFFAOYSA-N
Formula:	C17H24O4
SMILES:	<chem>C=CCC(C=C)OC(=O)CCCC(=O)OC(C=C)CC=C</chem>
Mol. weight [g/mol]:	292.37

Physical Properties

Property code	Value	Unit	Source
gf	-29.10	kJ/mol	Joback Method
hf	-392.65	kJ/mol	Joback Method
hfus	33.19	kJ/mol	Joback Method
hvap	68.29	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	3.504		Crippen Method
mcvol	248.070	ml/mol	McGowan Method
pc	1509.33	kPa	Joback Method
rinpol	1783.00		NIST Webbook
rinpol	1783.00		NIST Webbook
tb	726.78	K	Joback Method
tc	914.57	K	Joback Method
tf	388.63	K	Joback Method
vc	0.948	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	692.22	J/mol×K	726.78	Joback Method
cpg	760.28	J/mol×K	883.28	Joback Method
cpg	748.29	J/mol×K	851.98	Joback Method
cpg	735.52	J/mol×K	820.68	Joback Method
cpg	721.93	J/mol×K	789.38	Joback Method
cpg	707.51	J/mol×K	758.08	Joback Method
cpg	771.50	J/mol×K	914.57	Joback Method
dvisc	0.0000868	Paxs	726.78	Joback Method

dvisc	0.0001153	Paxs	670.42	Joback Method
dvisc	0.0001616	Paxs	614.06	Joback Method
dvisc	0.0002423	Paxs	557.70	Joback Method
dvisc	0.0003981	Paxs	501.35	Joback Method
dvisc	0.0007417	Paxs	444.99	Joback Method
dvisc	0.0016549	Paxs	388.63	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=U405292&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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