

Glutaric acid, ethyl hexa-1,5-dien-3-yl ester

Inchi:	InChI=1S/C13H20O4/c1-4-8-11(5-2)17-13(15)10-7-9-12(14)16-6-3/h4-5,11H,1-2,6-10H2
InchiKey:	JSIQLTYBHIMNNN-UHFFFAOYSA-N
Formula:	C13H20O4
SMILES:	C=CCC(C=C)OC(=O)CCCC(=O)OCC
Mol. weight [g/mol]:	240.30

Physical Properties

Property code	Value	Unit	Source
gf	-236.02	kJ/mol	Joback Method
hf	-555.67	kJ/mol	Joback Method
hfus	28.92	kJ/mol	Joback Method
hvap	61.12	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	2.394		Crippen Method
mvol	200.310	ml/mol	McGowan Method
pc	1920.30	kPa	Joback Method
rinpol	1520.00		NIST Webbook
rinpol	1520.00		NIST Webbook
tb	642.34	K	Joback Method
tc	826.69	K	Joback Method
tf	362.07	K	Joback Method
vc	0.767	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	523.93	J/molxK	642.34	Joback Method
cpg	538.22	J/molxK	673.06	Joback Method
cpg	551.81	J/molxK	703.79	Joback Method
cpg	564.71	J/molxK	734.51	Joback Method
cpg	576.92	J/molxK	765.24	Joback Method
cpg	588.46	J/molxK	795.96	Joback Method
cpg	599.33	J/molxK	826.69	Joback Method
dvisc	0.0019034	Paxs	362.07	Joback Method

dvisc	0.0009570	Paxs	408.78	Joback Method
dvisc	0.0005541	Paxs	455.49	Joback Method
dvisc	0.0003551	Paxs	502.21	Joback Method
dvisc	0.0002455	Paxs	548.92	Joback Method
dvisc	0.0001798	Paxs	595.63	Joback Method
dvisc	0.0001378	Paxs	642.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405293&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
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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