

Glutaric acid, 3-methylbut-2-yl oct-3-en-2-yl ester

Inchi:	InChI=1S/C18H32O4/c1-6-7-8-9-11-15(4)21-17(19)12-10-13-18(20)22-16(5)14(2)3/h9,11
InchiKey:	BZAQHJVZGCTKGM-PKNCBQFBNSA-N
Formula:	C18H32O4
SMILES:	CCCCC=CC(C)OC(=O)CCCC(=O)OC(C)C(C)C
Mol. weight [g/mol]:	312.44

Physical Properties

Property code	Value	Unit	Source
gf	-294.26	kJ/mol	Joback Method
hf	-803.07	kJ/mol	Joback Method
hfus	37.58	kJ/mol	Joback Method
hvap	72.77	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	4.423		Crippen Method
mcvol	275.060	ml/mol	McGowan Method
pc	1295.79	kPa	Joback Method
rinpol	1945.00		NIST Webbook
rinpol	1945.00		NIST Webbook
tb	766.66	K	Joback Method
tc	953.78	K	Joback Method
tf	386.86	K	Joback Method
vc	1.054	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	826.70	J/mol×K	766.66	Joback Method
cpg	904.02	J/mol×K	922.60	Joback Method
cpg	890.41	J/mol×K	891.41	Joback Method
cpg	875.90	J/mol×K	860.22	Joback Method
cpg	860.45	J/mol×K	829.03	Joback Method
cpg	844.06	J/mol×K	797.85	Joback Method
cpg	916.75	J/mol×K	953.78	Joback Method
dvisc	0.0000478	Paxs	766.66	Joback Method

dvisc	0.0000667	Paxs	703.36	Joback Method
dvisc	0.0000993	Paxs	640.06	Joback Method
dvisc	0.0001613	Paxs	576.76	Joback Method
dvisc	0.0002955	Paxs	513.46	Joback Method
dvisc	0.0006417	Paxs	450.16	Joback Method
dvisc	0.0017961	Paxs	386.86	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393985&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.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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