

Glutaric acid, ethyl 3-oxobut-2-yl ester

Inchi:	InChI=1S/C11H18O5/c1-4-15-10(13)6-5-7-11(14)16-9(3)8(2)12/h9H,4-7H2,1-3H3
InchiKey:	JYIIATMIXBDCJC-UHFFFAOYSA-N
Formula:	C11H18O5
SMILES:	CCOC(=O)CCCC(=O)OC(C)C(C)=O
Mol. weight [g/mol]:	230.26

Physical Properties

Property code	Value	Unit	Source
gf	-557.46	kJ/mol	Joback Method
hf	-877.83	kJ/mol	Joback Method
hfus	27.90	kJ/mol	Joback Method
hvap	64.75	kJ/mol	Joback Method
log10ws	-1.54		Crippen Method
logp	1.241		Crippen Method
mcvol	182.300	ml/mol	McGowan Method
pc	2244.00	kPa	Joback Method
rinpol	1571.00		NIST Webbook
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tb	657.09	K	Joback Method
tc	846.15	K	Joback Method
tf	392.98	K	Joback Method
vc	0.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	484.73	J/molxK	657.09	Joback Method
cpg	543.77	J/molxK	814.64	Joback Method
cpg	533.31	J/molxK	783.13	Joback Method
cpg	522.17	J/molxK	751.62	Joback Method
cpg	510.36	J/molxK	720.11	Joback Method
cpg	497.88	J/molxK	688.60	Joback Method
cpg	553.55	J/molxK	846.15	Joback Method
dvisc	0.0001586	Paxs	657.09	Joback Method

dvisc	0.0002055	Paxs	613.07	Joback Method
dvisc	0.0002770	Paxs	569.05	Joback Method
dvisc	0.0003925	Paxs	525.04	Joback Method
dvisc	0.0005929	Paxs	481.02	Joback Method
dvisc	0.0009733	Paxs	437.00	Joback Method
dvisc	0.0017853	Paxs	392.98	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=U359700&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
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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