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
rinpol	1571.00		NIST Webbook
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/mol×K	657.09	Joback Method
cpg	543.77	J/mol×K	814.64	Joback Method
cpg	533.31	J/mol×K	783.13	Joback Method
cpg	522.17	J/mol×K	751.62	Joback Method
cpg	510.36	J/mol×K	720.11	Joback Method
cpg	497.88	J/mol×K	688.60	Joback Method
cpg	553.55	J/mol×K	846.15	Joback Method
dvisc	0.0001586	Pa×s	657.09	Joback Method

dvisc	0.0002055	Pa×s	613.07	Joback Method
dvisc	0.0002770	Pa×s	569.05	Joback Method
dvisc	0.0003925	Pa×s	525.04	Joback Method
dvisc	0.0005929	Pa×s	481.02	Joback Method
dvisc	0.0009733	Pa×s	437.00	Joback Method
dvisc	0.0017853	Pa×s	392.98	Joback Method

Sources

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
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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