Succinic acid, ethyl 2-methylpent-3-yl ester

Inchi: InChI=1S/C12H22O4/c1-5-10(9(3)4)16-12(14)8-7-11(13)15-6-2/h9-10H,5-8H2,1-4H3
InchiKey: GCBUWOIPOZOTHT-UHFFFAOYSA-N
Formula: C12H22O4
SMILES: CCOC(=O)CCC(=O)OC(CC)C(C)C
Mol. weight [g/mol]: 230.30

Physical Properties

Property code	Value	Unit	Source
gf	-422.56	kJ/mol	Joback Method
hf	-791.17	kJ/mol	Joback Method
hfus	25.36	kJ/mol	Joback Method
hvap	59.84	kJ/mol	Joback Method
log10ws	-2.44		Crippen Method
logp	2.308		Crippen Method
mcvol	194.820	ml/mol	McGowan Method
pc	1954.41	kPa	Joback Method
rinpol	1458.00		NIST Webbook
rinpol	1458.00		NIST Webbook
tb	625.66	K	Joback Method
tc	808.87	K	Joback Method
tf	339.32	K	Joback Method
vc	0.744	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	516.81	J/mol×K	625.66	Joback Method
cpg	531.92	J/mol×K	656.19	Joback Method
cpg	546.34	J/mol×K	686.73	Joback Method
cpg	560.07	J/mol×K	717.26	Joback Method
cpg	573.11	J/mol×K	747.80	Joback Method
cpg	585.47	J/mol×K	778.33	Joback Method
cpg	597.13	J/mol×K	808.87	Joback Method
dvisc	0.0027555	Pa×s	339.32	Joback Method

dvisc	0.0012154	Pa×s	387.04	Joback Method
dvisc	0.0006416	Pa×s	434.77	Joback Method
dvisc	0.0003843	Pa×s	482.49	Joback Method
dvisc	0.0002525	Pa×s	530.21	Joback Method
dvisc	0.0001778	Pa×s	577.94	Joback Method
dvisc	0.0001321	Pa×s	625.66	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=U349382&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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