ethyl 3-methylbutyl succinate

Other names:	Ethyl isopentyl succinate
	Butanedioic acid, ethyl-(3-methyl-1-butyl) ester
Inchi:	InChI=1S/C11H20O4/c1-4-14-10(12)5-6-11(13)15-8-7-9(2)3/h9H,4-8H2,1-3H3
InchiKey:	GCXHTVAWZRIFAV-UHFFFAOYSA-N
Formula:	C11H20O4
SMILES:	CCOC(=O)CCC(=O)OCCC(C)C
Mol. weight [g/mol]:	216.27
CAS:	28024-16-0

Physical Properties

Property code	Value	Unit	Source
gf	-428.54	kJ/mol	Joback Method
hf	-765.25	kJ/mol	Joback Method
hfus	26.30	kJ/mol	Joback Method
hvap	58.00	kJ/mol	Joback Method
log10ws	-1.91		Crippen Method
logp	1.919		Crippen Method
mcvol	180.730	ml/mol	McGowan Method
pc	2115.83	kPa	Joback Method
rinpol	1451.00		NIST Webbook
rinpol	1421.00		NIST Webbook
rinpol	1421.00		NIST Webbook
rinpol	1423.00		NIST Webbook
rinpol	1432.60		NIST Webbook
rinpol	1430.00		NIST Webbook
rinpol	1432.60		NIST Webbook
rinpol	1451.00		NIST Webbook
rinpol	1454.00		NIST Webbook
rinpol	1436.00		NIST Webbook
rinpol	1436.00		NIST Webbook
ripol	1928.00		NIST Webbook
ripol	1901.00		NIST Webbook
ripol	1928.00		NIST Webbook
ripol	1892.00		NIST Webbook
ripol	1901.00		NIST Webbook
ripol	1892.00		NIST Webbook
tb	603.22	K	Joback Method

tc	784.89	K	Joback Method
tf	343.05	K	Joback Method
vc	0.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	465.43	J/mol×K	603.22	Joback Method
cpg	479.63	J/mol×K	633.50	Joback Method
cpg	493.21	J/mol×K	663.78	Joback Method
cpg	506.18	J/mol×K	694.06	Joback Method
cpg	518.53	J/mol×K	724.34	Joback Method
cpg	530.27	J/mol×K	754.61	Joback Method
cpg	541.38	J/mol×K	784.89	Joback Method
dvisc	0.0022861	Pa×s	343.05	Joback Method
dvisc	0.0011425	Pa×s	386.41	Joback Method
dvisc	0.0006567	Pa×s	429.77	Joback Method
dvisc	0.0004178	Pa×s	473.13	Joback Method
dvisc	0.0002868	Pa×s	516.50	Joback Method
dvisc	0.0002087	Pa×s	559.86	Joback Method
dvisc	0.0001589	Pa×s	603.22	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=C28024160&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume