ethyl isobutyl succinate

Other names: Ethyl 2-methylpropyl succinate
Inchi: InChI=1S/C10H18O4/c1-4-13-9(11)5-6-10(12)14-7-8(2)3/h8H,4-7H2,1-3H3
InchiKey: ITMHQIWFDVCNJS-UHFFFAOYSA-N
Formula: C10H18O4
SMILES: CCOC(=O)CCC(=O)OCC(C)C
Mol. weight [g/mol]: 202.25

Physical Properties

Property code	Value	Unit	Source
gf	-436.96	kJ/mol	Joback Method
hf	-744.61	kJ/mol	Joback Method
hfus	23.71	kJ/mol	Joback Method
hvap	55.78	kJ/mol	Joback Method
log10ws	-1.49		Crippen Method
logp	1.529		Crippen Method
mcvol	166.640	ml/mol	McGowan Method
pc	2315.84	kPa	Joback Method
rinpol	1330.00		NIST Webbook
rinpol	1324.00		NIST Webbook
ripol	1791.00		NIST Webbook
ripol	1785.00		NIST Webbook
ripol	1793.00		NIST Webbook
ripol	1785.00		NIST Webbook
ripol	1791.00		NIST Webbook
ripol	1785.00		NIST Webbook
tb	580.34	K	Joback Method
tc	763.73	K	Joback Method
tf	331.78	K	Joback Method
vc	0.637	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	416.07	J/mol×K	580.34	Joback Method

cpg	477.83	J/mol×K	733.16	Joback Method
cpg	466.62	J/mol×K	702.60	Joback Method
cpg	454.83	J/mol×K	672.03	Joback Method
cpg	442.48	J/mol×K	641.47	Joback Method
cpg	429.55	J/mol×K	610.90	Joback Method
cpg	488.46	J/mol×K	763.73	Joback Method
dvisc	0.0001771	Pa×s	580.34	Joback Method
dvisc	0.0002316	Pa×s	538.91	Joback Method
dvisc	0.0003168	Pa×s	497.49	Joback Method
dvisc	0.0004587	Pa×s	456.06	Joback Method
dvisc	0.0007150	Pa×s	414.63	Joback Method
dvisc	0.0012300	Pa×s	373.21	Joback Method
dvisc	0.0024229	Pa×s	331.78	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=R319201&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

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