Succinic acid, 3-methyl-2-butyl 2-pentyl ester

Other names: Succinic acid, 2-methyl-3-pentyl 2-pentyl ester
Inchi: InChI=1S/C14H26O4/c1-6-7-11(4)17-13(15)8-9-14(16)18-12(5)10(2)3/h10-12H,6-9H2,1-5
InchiKey: JONOCWHTZOAQQC-UHFFFAOYSA-N
Formula: C14H26O4
SMILES: CCCC(C)OC(=O)CCC(=O)OC(C)C(C)C
Mol. weight [g/mol]: 258.35

Physical Properties

Property code	Value	Unit	Source
gf	-408.16	kJ/mol	Joback Method
hf	-837.73	kJ/mol	Joback Method
hfus	27.02	kJ/mol	Joback Method
hvap	63.91	kJ/mol	Joback Method
log10ws	-3.39		Crippen Method
logp	3.086		Crippen Method
mcvol	223.000	ml/mol	McGowan Method
pc	1671.43	kPa	Joback Method
rinpol	1632.00		NIST Webbook
tb	670.98	K	Joback Method
tc	854.46	K	Joback Method
tf	346.86	K	Joback Method
vc	0.850	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	623.56	J/mol×K	670.98	Joback Method
cpg	639.97	J/mol×K	701.56	Joback Method
cpg	655.56	J/mol×K	732.14	Joback Method
cpg	670.35	J/mol×K	762.72	Joback Method
cpg	684.34	J/mol×K	793.30	Joback Method
cpg	697.54	J/mol×K	823.88	Joback Method
cpg	709.94	J/mol×K	854.46	Joback Method
dvisc	0.0030168	Pa×s	346.86	Joback Method

dvisc	0.0011517	Pa×s	400.88	Joback Method
dvisc	0.0005527	Pa×s	454.90	Joback Method
dvisc	0.0003099	Pa×s	508.92	Joback Method
dvisc	0.0001942	Pa×s	562.94	Joback Method
dvisc	0.0001321	Pa×s	616.96	Joback Method
dvisc	0.0000956	Pa×s	670.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370896&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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