Succinic acid, heptyl 6-methylhept-2-yl ester

Inchi: InChI=1S/C19H36O4/c1-5-6-7-8-9-15-22-18(20)13-14-19(21)23-17(4)12-10-11-16(2)3/h1
InchiKey: GQCUTEMOIMVBER-UHFFFAOYSA-N
Formula: C19H36O4
SMILES: CCCCCCCOC(=O)CCC(=O)OC(C)CCCC(C)C
Mol. weight [g/mol]: 328.49

Physical Properties

Property code	Value	Unit	Source
gf	-363.62	kJ/mol	Joback Method
hf	-935.65	kJ/mol	Joback Method
hfus	43.49	kJ/mol	Joback Method
hvap	75.42	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	5.038		Crippen Method
mcvol	293.450	ml/mol	McGowan Method
pc	1161.66	kPa	Joback Method
rinpol	2118.00		NIST Webbook
rinpol	2118.00		NIST Webbook
tb	785.82	K	Joback Method
tc	968.88	K	Joback Method
tf	418.21	K	Joback Method
vc	1.135	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	909.87	J/mol×K	785.82	Joback Method
cpg	927.92	J/mol×K	816.33	Joback Method
cpg	944.96	J/mol×K	846.84	Joback Method
cpg	961.00	J/mol×K	877.35	Joback Method
cpg	976.05	J/mol×K	907.86	Joback Method
cpg	990.13	J/mol×K	938.37	Joback Method
cpg	1003.26	J/mol×K	968.88	Joback Method
dvisc	0.0013492	Pa×s	418.21	Joback Method

dvisc	0.0005543	Pa×s	479.48	Joback Method
dvisc	0.0002785	Pa×s	540.75	Joback Method
dvisc	0.0001610	Pa×s	602.01	Joback Method
dvisc	0.0001030	Pa×s	663.28	Joback Method
dvisc	0.0000711	Pa×s	724.55	Joback Method
dvisc	0.0000520	Pa×s	785.82	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=U381366&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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