Succinic acid, butyl 10-chlorodecyl ester

Inchi: InChI=1S/C18H33ClO4/c1-2-3-15-22-17(20)12-13-18(21)23-16-11-9-7-5-4-6-8-10-14-19/
InchiKey: LMHBNPLNRUVHBM-UHFFFAOYSA-N
Formula: C18H33ClO4
SMILES: CCCCOC(=O)CCC(=O)OCCCCCCCCCCCCl
Mol. weight [g/mol]: 348.90

Physical Properties

Property code	Value	Unit	Source
gf	-379.09	kJ/mol	Joback Method
hf	-920.19	kJ/mol	Joback Method
hfus	52.15	kJ/mol	Joback Method
hvap	78.36	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	5.013		Crippen Method
mcvol	291.600	ml/mol	McGowan Method
pc	1196.48	kPa	Joback Method
rinpol	2457.00		NIST Webbook
rinpol	2457.00		NIST Webbook
tb	801.25	K	Joback Method
tc	986.02	K	Joback Method
tf	466.86	K	Joback Method
vc	1.141	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	881.08	J/mol×K	801.25	Joback Method
cpg	897.61	J/mol×K	832.05	Joback Method
cpg	913.18	J/mol×K	862.84	Joback Method
cpg	927.81	J/mol×K	893.64	Joback Method
cpg	941.51	J/mol×K	924.43	Joback Method
cpg	954.29	J/mol×K	955.23	Joback Method
cpg	966.18	J/mol×K	986.02	Joback Method
dvisc	0.0008274	Pa×s	466.86	Joback Method

dvisc	0.0004253	Pa×s	522.59	Joback Method
dvisc	0.0002486	Pa×s	578.32	Joback Method
dvisc	0.0001596	Pa×s	634.06	Joback Method
dvisc	0.0001101	Pa×s	689.79	Joback Method
dvisc	0.0000803	Pa×s	745.52	Joback Method
dvisc	0.0000612	Pa×s	801.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U349185&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

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