Succinic acid, 8-chlorooctyl 3,3-dimethylbut-2-yl ester

Inchi: InChI=1S/C18H33ClO4/c1-15(18(2,3)4)23-17(21)12-11-16(20)22-14-10-8-6-5-7-9-13-19/

InchiKey: QPYRTANJGLFMFW-UHFFFAOYSA-N

Formula: C18H33ClO4

SMILES: CC(OC(=O)CCC(=O)OCCCCCCCCCCl)C(C)(C)C

Mol. weight [g/mol]: 348.90

Physical Properties

Property code	Value	Unit	Source
gf	-378.69	kJ/mol	Joback Method
hf	-934.22	kJ/mol	Joback Method
hfus	41.21	kJ/mol	Joback Method
hvap	76.67	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.867		Crippen Method
mcvol	291.600	ml/mol	McGowan Method
pc	1219.14	kPa	Joback Method
rinpol	2331.00		NIST Webbook
rinpol	2331.00		NIST Webbook
tb	797.58	K	Joback Method
tc	987.12	K	Joback Method
tf	454.28	K	Joback Method
vc	1.123	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	882.88	J/mol×K	797.58	Joback Method
cpg	899.59	J/mol×K	829.17	Joback Method
cpg	915.30	J/mol×K	860.76	Joback Method
cpg	930.02	J/mol×K	892.35	Joback Method
cpg	943.81	J/mol×K	923.94	Joback Method
cpg	956.67	J/mol×K	955.53	Joback Method
cpg	968.64	J/mol×K	987.12	Joback Method
dvisc	0.0009306	Pa×s	454.28	Joback Method

dvisc	0.0004241	Pa×s	511.50	Joback Method
dvisc	0.0002264	Pa×s	568.71	Joback Method
dvisc	0.0001355	Pa×s	625.93	Joback Method
dvisc	0.0000884	Pa×s	683.15	Joback Method
dvisc	0.0000616	Pa×s	740.36	Joback Method
dvisc	0.0000452	Pa×s	797.58	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=U390632&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