

Succinic acid, 8-chlorooctyl 4-methylpent-2-yl ester

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

Physical Properties

Property code	Value	Unit	Source
gf	-383.97	kJ/mol	Joback Method
hf	-930.75	kJ/mol	Joback Method
hfus	45.10	kJ/mol	Joback Method
hvap	77.58	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.867		Crippen Method
mcvol	291.600	ml/mol	McGowan Method
pc	1209.83	kPa	Joback Method
rinpol	2319.00		NIST Webbook
rinpol	2319.00		NIST Webbook
tb	800.37	K	Joback Method
tc	987.50	K	Joback Method
tf	436.86	K	Joback Method
vc	1.129	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	882.09	J/molxK	800.37	Joback Method
cpg	898.84	J/molxK	831.56	Joback Method
cpg	914.58	J/molxK	862.75	Joback Method
cpg	929.34	J/molxK	893.93	Joback Method
cpg	943.13	J/molxK	925.12	Joback Method
cpg	955.96	J/molxK	956.31	Joback Method
cpg	967.85	J/molxK	987.50	Joback Method
dvisc	0.0011551	Paxs	436.86	Joback Method

dvisc	0.0005021	Paxs	497.44	Joback Method
dvisc	0.0002615	Paxs	558.03	Joback Method
dvisc	0.0001548	Paxs	618.62	Joback Method
dvisc	0.0001006	Paxs	679.20	Joback Method
dvisc	0.0000701	Paxs	739.79	Joback Method
dvisc	0.0000517	Paxs	800.37	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U390436&Units=SI

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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