Succinic acid, 8-chlorooctyl neopentyl ester

Inchi: InChI=1S/C17H31ClO4/c1-17(2,3)14-22-16(20)11-10-15(19)21-13-9-7-5-4-6-8-12-18/h4-
InchiKey: RGZOMDFDFBOKEB-UHFFFAOYSA-N
Formula: C17H31ClO4
SMILES: CC(C)(C)COC(=O)CCC(=O)OCCCCCCCCCl
Mol. weight [g/mol]: 334.88

Physical Properties

Property code	Value	Unit	Source
gf	-384.67	kJ/mol	Joback Method
hf	-908.30	kJ/mol	Joback Method
hfus	42.14	kJ/mol	Joback Method
hvap	74.84	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	4.478		Crippen Method
mcvol	277.510	ml/mol	McGowan Method
pc	1297.66	kPa	Joback Method
rinpol	2264.00		NIST Webbook
rinpol	2264.00		NIST Webbook
tb	775.14	K	Joback Method
tc	962.10	K	Joback Method
tf	458.01	K	Joback Method
vc	1.073	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	824.05	J/mol×K	775.14	Joback Method
cpg	840.29	J/mol×K	806.30	Joback Method
cpg	855.58	J/mol×K	837.46	Joback Method
cpg	869.97	J/mol×K	868.62	Joback Method
cpg	883.46	J/mol×K	899.78	Joback Method
cpg	896.10	J/mol×K	930.94	Joback Method
cpg	907.89	J/mol×K	962.10	Joback Method
dvisc	0.0008822	Pa×s	458.01	Joback Method

dvisc	0.0004420	Pa×s	510.86	Joback Method
dvisc	0.0002521	Pa×s	563.72	Joback Method
dvisc	0.0001583	Pa×s	616.57	Joback Method
dvisc	0.0001070	Pa×s	669.43	Joback Method
dvisc	0.0000766	Pa×s	722.28	Joback Method
dvisc	0.0000574	Pa×s	775.14	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389590&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

Latest version available from:
https://www.chemeo.com/cid/114-597-3/Succinic-acid-8-chlorooctyl-neopentyl-ester.pdf
Generated by Cheméo on 2024-04-29 00:08:08.32477336 +0000 UTC m=+16638537.245350688.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.