

Succinic acid, dodec-2-en-1-yl 10-chlorodecyl ester

Inchi:	InChI=1S/C26H47ClO4/c1-2-3-4-5-6-7-9-12-15-18-23-30-25(28)20-21-26(29)31-24-19-10
InchiKey:	KHYPPIMXXBFFAH-OBGWFSINSA-N
Formula:	C26H47ClO4
SMILES:	CCCCCCCCC=CCOC(=O)CCC(=O)OCCCCCCCCCl
Mol. weight [g/mol]:	459.10

Physical Properties

Property code	Value	Unit	Source
gf	-231.51	kJ/mol	Joback Method
hf	-968.09	kJ/mol	Joback Method
hfus	73.07	kJ/mol	Joback Method
hvap	96.12	kJ/mol	Joback Method
log10ws	-8.44		Crippen Method
logp	7.909		Crippen Method
mcvol	400.020	ml/mol	McGowan Method
pc	768.61	kPa	Joback Method
rinpol	3281.00		NIST Webbook
tb	988.45	K	Joback Method
tc	1218.40	K	Joback Method
tf	551.94	K	Joback Method
vc	1.569	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1347.25	J/molxK	988.45	Joback Method
cpg	1367.17	J/molxK	1026.77	Joback Method
cpg	1385.52	J/molxK	1065.10	Joback Method
cpg	1402.37	J/molxK	1103.42	Joback Method
cpg	1417.79	J/molxK	1141.75	Joback Method
cpg	1431.87	J/molxK	1180.07	Joback Method
cpg	1444.68	J/molxK	1218.40	Joback Method
dvisc	0.0002914	Paxs	551.94	Joback Method
dvisc	0.0001351	Paxs	624.69	Joback Method

dvisc	0.0000735	Paxs	697.44	Joback Method
dvisc	0.0000449	Paxs	770.19	Joback Method
dvisc	0.0000299	Paxs	842.95	Joback Method
dvisc	0.0000212	Paxs	915.70	Joback Method
dvisc	0.0000158	Paxs	988.45	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=U390419&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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