

Succinic acid, 8-chlorooctyl 2,4-dimethylpent-3-yl ester

Inchi:	InChI=1S/C19H35ClO4/c1-15(2)19(16(3)4)24-18(22)12-11-17(21)23-14-10-8-6-5-7-9-13
InchiKey:	OULQSKGXULWUSP-UHFFFAOYSA-N
Formula:	C19H35ClO4
SMILES:	CC(C)C(OC(=O)CCC(=O)OCCCCCCCCCl)C(C)C
Mol. weight [g/mol]:	362.93

Physical Properties

Property code	Value	Unit	Source
gf	-377.99	kJ/mol	Joback Method
hf	-956.67	kJ/mol	Joback Method
hfus	44.17	kJ/mol	Joback Method
hvap	79.42	kJ/mol	Joback Method
log10ws	-5.28		Crippen Method
logp	5.113		Crippen Method
mvol	305.690	ml/mol	McGowan Method
pc	1139.03	kPa	Joback Method
rinpol	2550.00		NIST Webbook
rinpol	2550.00		NIST Webbook
tb	822.81	K	Joback Method
tc	1013.05	K	Joback Method
tf	433.13	K	Joback Method
vc	1.179	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	942.04	J/molxK	822.81	Joback Method
cpg	959.23	J/molxK	854.52	Joback Method
cpg	975.33	J/molxK	886.22	Joback Method
cpg	990.36	J/molxK	917.93	Joback Method
cpg	1004.36	J/molxK	949.64	Joback Method
cpg	1017.32	J/molxK	981.34	Joback Method
cpg	1029.28	J/molxK	1013.05	Joback Method
dvisc	0.0012389	Paxs	433.13	Joback Method

dvisc	0.0004842	Paxs	498.08	Joback Method
dvisc	0.0002350	Paxs	563.02	Joback Method
dvisc	0.0001325	Paxs	627.97	Joback Method
dvisc	0.0000831	Paxs	692.92	Joback Method
dvisc	0.0000565	Paxs	757.86	Joback Method
dvisc	0.0000408	Paxs	822.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390513&Units=SI
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

Legend

cp_g:	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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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/99-663-7/Succinic-acid-8-chlorooctyl-2-4-dimethylpent-3-yl-ester.pdf>

Generated by Cheméo on 2024-05-03 03:40:31.946214066 +0000 UTC m=+16996880.866791378.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.