

Succinic acid, 8-chlorooctyl heptyl ester

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

Physical Properties

Property code	Value	Unit	Source
gf	-370.67	kJ/mol	Joback Method
hf	-940.83	kJ/mol	Joback Method
hfus	54.74	kJ/mol	Joback Method
hvap	80.58	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	5.403		Crippen Method
mvol	305.690	ml/mol	McGowan Method
pc	1120.80	kPa	Joback Method
rinpol	2553.00		NIST Webbook
tb	824.13	K	Joback Method
tc	1011.58	K	Joback Method
tf	478.13	K	Joback Method
vc	1.196	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	940.55	J/molxK	824.13	Joback Method
cpg	957.49	J/molxK	855.37	Joback Method
cpg	973.41	J/molxK	886.61	Joback Method
cpg	988.32	J/molxK	917.85	Joback Method
cpg	1002.25	J/molxK	949.09	Joback Method
cpg	1015.20	J/molxK	980.33	Joback Method
cpg	1027.20	J/molxK	1011.58	Joback Method
dvisc	0.0007414	Paxs	478.13	Joback Method
dvisc	0.0003768	Paxs	535.80	Joback Method

dvisc	0.0002184	Paxs	593.46	Joback Method
dvisc	0.0001394	Paxs	651.13	Joback Method
dvisc	0.0000957	Paxs	708.80	Joback Method
dvisc	0.0000696	Paxs	766.46	Joback Method
dvisc	0.0000529	Paxs	824.13	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=U349291&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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