Succinic acid, 8-chlorooctyl 2-ethoxyethyl ester

Inchi: InChI=1S/C16H29ClO5/c1-2-20-13-14-22-16(19)10-9-15(18)21-12-8-6-4-3-5-7-11-17/h2-

InchiKey: UAGRVZMKTLMYDD-UHFFFAOYSA-N

Formula: C16H29ClO5

SMILES: CCOCCOC(=O)CCC(=O)OCCCCCCCCCl

Mol. weight [g/mol]: 336.85

Physical Properties

Property code	Value	Unit	Source
gf	-500.93	kJ/mol	Joback Method
hf	-1011.13	kJ/mol	Joback Method
hfus	48.16	kJ/mol	Joback Method
hvap	76.32	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	3.469		Crippen Method
mcvol	269.290	ml/mol	McGowan Method
pc	1355.63	kPa	Joback Method
rinpol	2359.00		NIST Webbook
rinpol	2359.00		NIST Webbook
tb	777.91	K	Joback Method
tc	961.04	K	Joback Method
tf	466.55	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	794.26	J/mol×K	777.91	Joback Method
cpg	809.77	J/mol×K	808.43	Joback Method
cpg	824.37	J/mol×K	838.95	Joback Method
cpg	838.08	J/mol×K	869.48	Joback Method
cpg	850.89	J/mol×K	900.00	Joback Method
cpg	862.81	J/mol×K	930.52	Joback Method
cpg	873.83	J/mol×K	961.04	Joback Method
dvisc	0.0007044	Pa×s	466.55	Joback Method

dvisc	0.0003824	Pa×s	518.44	Joback Method
dvisc	0.0002320	Pa×s	570.34	Joback Method
dvisc	0.0001530	Pa×s	622.23	Joback Method
dvisc	0.0001076	Pa×s	674.12	Joback Method
dvisc	0.0000796	Pa×s	726.02	Joback Method
dvisc	0.0000612	Pa×s	777.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390672&Units=SI
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

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