

Succinic acid, 8-chlorooctyl tetrahydrofurfuryl ester

Inchi: InChI=1S/C17H29ClO5/c18-11-5-3-1-2-4-6-12-22-16(19)9-10-17(20)23-14-15-8-7-13-21-20
InchiKey: RPOFSNZQGXXQAKX-UHFFFAOYSA-N
Formula: C17H29ClO5
SMILES: O=C(CCC(=O)OCC1CCCO1)OCCCCCCCCCI
Mol. weight [g/mol]: 348.86

Physical Properties

Property code	Value	Unit	Source
gf	-437.08	kJ/mol	Joback Method
hf	-971.07	kJ/mol	Joback Method
hfus	51.47	kJ/mol	Joback Method
hvap	80.90	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	3.611		Crippen Method
mcvol	272.520	ml/mol	McGowan Method
pc	1452.35	kPa	Joback Method
rinpol	2658.00		NIST Webbook
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tb	820.60	K	Joback Method
tc	1017.74	K	Joback Method
tf	493.06	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	847.61	J/mol×K	820.60	Joback Method
cpg	917.40	J/mol×K	984.88	Joback Method
cpg	905.56	J/mol×K	952.02	Joback Method
cpg	892.68	J/mol×K	919.17	Joback Method
cpg	878.75	J/mol×K	886.31	Joback Method
cpg	863.73	J/mol×K	853.46	Joback Method
cpg	928.22	J/mol×K	1017.74	Joback Method
dvisc	0.0000901	Pa×s	820.60	Joback Method

dvisc	0.0001164	Pa×s	766.01	Joback Method
dvisc	0.0001566	Pa×s	711.42	Joback Method
dvisc	0.0002211	Pa×s	656.83	Joback Method
dvisc	0.0003326	Pa×s	602.24	Joback Method
dvisc	0.0005426	Pa×s	547.65	Joback Method
dvisc	0.0009864	Pa×s	493.06	Joback Method

Sources

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=U390726&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log_{10ws}:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
rin_{pol}:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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