Succinic acid, 4-chlorophenethyl heptadecyl ester

Inchi: InChI=1S/C29H47ClO4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-24-33-28(31)21-22-29(

InchiKey: BZEAKNCUMASPDS-UHFFFAOYSA-N

Formula: C29H47ClO4

SMILES: CCCCCCCCCCCCCCCCCCOC(=O)CCC(=O)OCCc1ccc(Cl)cc1

Mol. weight [g/mol]: 495.13

Physical Properties

Property code	Value	Unit	Source
gf	-183.69	kJ/mol	Joback Method
hf	-922.17	kJ/mol	Joback Method
hfus	74.29	kJ/mol	Joback Method
hvap	105.78	kJ/mol	Joback Method
log10ws	-9.47		Crippen Method
logp	8.620		Crippen Method
mcvol	422.830	ml/mol	McGowan Method
pc	758.49	kPa	Joback Method
rinpol	3559.00		NIST Webbook
rinpol	3559.00		NIST Webbook
tb	1084.59	K	Joback Method
tc	1341.47	K	Joback Method
tf	629.77	K	Joback Method
vc	1.649	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1458.02	J/mol×K	1084.59	Joback Method
cpg	1475.49	J/mol×K	1127.40	Joback Method
cpg	1490.93	J/mol×K	1170.22	Joback Method
cpg	1504.47	J/mol×K	1213.03	Joback Method
cpg	1516.20	J/mol×K	1255.85	Joback Method
cpg	1526.22	J/mol×K	1298.66	Joback Method
cpg	1534.64	J/mol×K	1341.47	Joback Method
dvisc	0.0001626	Pa×s	629.77	Joback Method

dvisc	0.0000832	Pa×s	705.57	Joback Method
dvisc	0.0000484	Pa×s	781.38	Joback Method
dvisc	0.0000310	Pa×s	857.18	Joback Method
dvisc	0.0000214	Pa×s	932.98	Joback Method
dvisc	0.0000156	Pa×s	1008.79	Joback Method
dvisc	0.0000119	Pa×s	1084.59	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381528&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

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