

Succinic acid, 4-chlorophenethyl octadecyl ester

Inchi:	InChI=1S/C30H49ClO4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-25-34-29(32)22-23
InchiKey:	FTACGNCTNZQYBC-UHFFFAOYSA-N
Formula:	C30H49ClO4
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)CCC(=O)OCCc1ccc(Cl)cc1
Mol. weight [g/mol]:	509.16

Physical Properties

Property code	Value	Unit	Source
gf	-175.27	kJ/mol	Joback Method
hf	-942.81	kJ/mol	Joback Method
hfus	76.88	kJ/mol	Joback Method
hvap	108.01	kJ/mol	Joback Method
log10ws	-9.89		Crippen Method
logp	9.011		Crippen Method
mcvol	436.920	ml/mol	McGowan Method
pc	719.91	kPa	Joback Method
rinpol	3658.00		NIST Webbook
rinpol	3658.00		NIST Webbook
tb	1107.47	K	Joback Method
tc	1376.24	K	Joback Method
tf	641.04	K	Joback Method
vc	1.704	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1521.36	J/molxK	1107.47	Joback Method
cpg	1539.23	J/molxK	1152.27	Joback Method
cpg	1554.91	J/molxK	1197.06	Joback Method
cpg	1568.52	J/molxK	1241.86	Joback Method
cpg	1580.19	J/molxK	1286.65	Joback Method
cpg	1590.03	J/molxK	1331.45	Joback Method
cpg	1598.18	J/molxK	1376.24	Joback Method
dvisc	0.0001423	Paxs	641.04	Joback Method

dvisc	0.0000721	Paxs	718.78	Joback Method
dvisc	0.0000418	Paxs	796.52	Joback Method
dvisc	0.0000266	Paxs	874.25	Joback Method
dvisc	0.0000183	Paxs	951.99	Joback Method
dvisc	0.0000133	Paxs	1029.73	Joback Method
dvisc	0.0000101	Paxs	1107.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381529&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

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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