

Succinic acid, 4-chloro-3-methylphenyl 3-pentyl ester

Inchi:	InChI=1S/C16H21ClO4/c1-4-12(5-2)20-15(18)8-9-16(19)21-13-6-7-14(17)11(3)10-13/h6-
InchiKey:	BYALCFPHUBNCBC-UHFFFAOYSA-N
Formula:	C16H21ClO4
SMILES:	CCC(CC)OC(=O)CCC(=O)Oc1ccc(Cl)c(C)c1
Mol. weight [g/mol]:	312.79

Physical Properties

Property code	Value	Unit	Source
gf	-305.22	kJ/mol	Joback Method
hf	-670.60	kJ/mol	Joback Method
hfus	36.71	kJ/mol	Joback Method
hvap	77.12	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	4.066		Crippen Method
mcvol	239.660	ml/mol	McGowan Method
pc	1750.67	kPa	Joback Method
rinsol	2129.00		NIST Webbook
tb	791.69	K	Joback Method
tc	1000.85	K	Joback Method
tf	480.78	K	Joback Method
vc	0.914	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	674.74	J/molxK	791.69	Joback Method
cpg	688.84	J/molxK	826.55	Joback Method
cpg	701.92	J/molxK	861.41	Joback Method
cpg	713.99	J/molxK	896.27	Joback Method
cpg	725.06	J/molxK	931.13	Joback Method
cpg	735.14	J/molxK	965.99	Joback Method
cpg	744.24	J/molxK	1000.85	Joback Method
dvisc	0.0006920	Paxs	480.78	Joback Method
dvisc	0.0004012	Paxs	532.60	Joback Method

dvisc	0.0002562	Paxs	584.42	Joback Method
dvisc	0.0001760	Paxs	636.24	Joback Method
dvisc	0.0001280	Paxs	688.05	Joback Method
dvisc	0.0000973	Paxs	739.87	Joback Method
dvisc	0.0000767	Paxs	791.69	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=U370917&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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