

Succinic acid, 4-chloro-3-methylphenyl trans-4-methylcyclohexyl ester

Inchi:	InChI=1S/C18H23ClO4/c1-12-3-5-14(6-4-12)22-17(20)9-10-18(21)23-15-7-8-16(19)13(2)
InchiKey:	YJONPWCLHGBIOL-UHFFFAOYSA-N
Formula:	C18H23ClO4
SMILES:	<chem>Cc1cc(OC(=O)CCC(=O)OC2CCC(C)CC2)ccc1Cl</chem>
Mol. weight [g/mol]:	338.83

Physical Properties

Property code	Value	Unit	Source
gf	-269.20	kJ/mol	Joback Method
hf	-672.62	kJ/mol	Joback Method
hfus	38.32	kJ/mol	Joback Method
hvap	82.08	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	4.456		Crippen Method
mvol	256.980	ml/mol	McGowan Method
pc	1710.36	kPa	Joback Method
rinpol	2513.00		NIST Webbook
rinpol	2513.00		NIST Webbook
tb	852.77	K	Joback Method
tc	1079.80	K	Joback Method
tf	521.46	K	Joback Method
vc	0.965	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	785.60	J/molxK	852.77	Joback Method
cpg	801.34	J/molxK	890.61	Joback Method
cpg	815.58	J/molxK	928.45	Joback Method
cpg	828.31	J/molxK	966.29	Joback Method
cpg	839.56	J/molxK	1004.13	Joback Method
cpg	849.33	J/molxK	1041.96	Joback Method
cpg	857.65	J/molxK	1079.80	Joback Method
dvisc	0.0006484	Paxs	521.46	Joback Method

dvisc	0.0003934	Paxs	576.68	Joback Method
dvisc	0.0002605	Paxs	631.90	Joback Method
dvisc	0.0001843	Paxs	687.12	Joback Method
dvisc	0.0001373	Paxs	742.33	Joback Method
dvisc	0.0001065	Paxs	797.55	Joback Method
dvisc	0.0000854	Paxs	852.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390072&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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