

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

Inchi:	InChI=1S/C19H19ClO5/c1-13-11-16(7-8-17(13)20)25-19(22)10-9-18(21)24-12-14-3-5-15
InchiKey:	YXFFZWIXZXWMCQ-UHFFFAOYSA-N
Formula:	C19H19ClO5
SMILES:	COc1ccc(COC(=O)CCC(=O)Oc2ccc(Cl)c(C)c2)cc1
Mol. weight [g/mol]:	362.80

Physical Properties

Property code	Value	Unit	Source
gf	-279.74	kJ/mol	Joback Method
hf	-634.40	kJ/mol	Joback Method
hfus	42.84	kJ/mol	Joback Method
hvap	89.53	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	4.086		Crippen Method
mvol	264.040	ml/mol	McGowan Method
pc	1755.07	kPa	Joback Method
rinpol	2900.00		NIST Webbook
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tb	914.85	K	Joback Method
tc	1144.37	K	Joback Method
tf	590.76	K	Joback Method
vc	0.999	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	770.95	J/molxK	914.85	Joback Method
cpg	782.68	J/molxK	953.10	Joback Method
cpg	793.04	J/molxK	991.36	Joback Method
cpg	802.03	J/molxK	1029.61	Joback Method
cpg	809.65	J/molxK	1067.86	Joback Method
cpg	815.92	J/molxK	1106.12	Joback Method
cpg	820.83	J/molxK	1144.37	Joback Method
dvisc	0.0002695	Paxs	590.76	Joback Method

dvisc	0.0001751	Paxs	644.77	Joback Method
dvisc	0.0001216	Paxs	698.79	Joback Method
dvisc	0.0000889	Paxs	752.80	Joback Method
dvisc	0.0000679	Paxs	806.82	Joback Method
dvisc	0.0000536	Paxs	860.83	Joback Method
dvisc	0.0000435	Paxs	914.85	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=U389695&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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