

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

Inchi: InChI=1S/C24H21ClO5/c1-17-14-21(10-11-22(17)25)30-24(27)13-12-23(26)28-16-18-6-5
InchiKey: ZZGKDILGUVTLHR-UHFFFAOYSA-N
Formula: C24H21ClO5
SMILES: Cc1cc(OC(=O)CCC(=O)OCc2cccc(Oc3ccccc3)c2)ccc1Cl
Mol. weight [g/mol]: 424.87

Physical Properties

Property code	Value	Unit	Source
gf	-125.23	kJ/mol	Joback Method
hf	-501.07	kJ/mol	Joback Method
hfus	49.83	kJ/mol	Joback Method
hvap	102.94	kJ/mol	Joback Method
log10ws	-6.81		Crippen Method
logp	5.870		Crippen Method
mcvol	310.730	ml/mol	McGowan Method
pc	1554.90	kPa	Joback Method
rinpol	3300.00		NIST Webbook
rinpol	3300.00		NIST Webbook
tb	1055.93	K	Joback Method
tc	1305.88	K	Joback Method
tf	673.53	K	Joback Method
vc	1.171	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	949.21	J/molxK	1055.93	Joback Method
cpg	958.05	J/molxK	1097.59	Joback Method
cpg	965.19	J/molxK	1139.25	Joback Method
cpg	970.70	J/molxK	1180.90	Joback Method
cpg	974.60	J/molxK	1222.56	Joback Method
cpg	976.96	J/molxK	1264.22	Joback Method
cpg	977.80	J/molxK	1305.88	Joback Method
dvisc	0.0001471	Paxs	673.53	Joback Method

dvisc	0.0000933	Paxs	737.26	Joback Method
dvisc	0.0000636	Paxs	801.00	Joback Method
dvisc	0.0000459	Paxs	864.73	Joback Method
dvisc	0.0000347	Paxs	928.46	Joback Method
dvisc	0.0000271	Paxs	992.20	Joback Method
dvisc	0.0000218	Paxs	1055.93	Joback Method

Sources

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=U390377&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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