Succinic acid, 8-chlorooctyl 3-phenoxybenzyl ester

Inchi: InChI=1S/C25H31ClO5/c26-17-8-3-1-2-4-9-18-29-24(27)15-16-25(28)30-20-21-11-10-14

InchiKey: VQTPZKFQKUYZLH-UHFFFAOYSA-N

Formula: C25H31ClO5

SMILES: O=C(CCC(=O)OCc1cccc(Oc2ccccc2)c1)OCCCCCCCCCl

Mol. weight [g/mol]: 446.96

Physical Properties

Property code	Value	Unit	Source
gf	-209.96	kJ/mol	Joback Method
hf	-735.30	kJ/mol	Joback Method
hfus	59.16	kJ/mol	Joback Method
hvap	101.56	kJ/mol	Joback Method
log10ws	-6.89		Crippen Method
logp	6.425		Crippen Method
mcvol	348.580	ml/mol	McGowan Method
pc	1162.45	kPa	Joback Method
rinpol	3384.00		NIST Webbook
rinpol	3384.00		NIST Webbook
tb	1042.17	K	Joback Method
tc	1276.60	K	Joback Method
tf	633.34	K	Joback Method
vc	1.335	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1125.70	J/mol×K	1042.17	Joback Method
cpg	1137.74	J/mol×K	1081.24	Joback Method
cpg	1148.17	J/mol×K	1120.31	Joback Method
cpg	1157.02	J/mol×K	1159.38	Joback Method
cpg	1164.35	J/mol×K	1198.46	Joback Method
cpg	1170.21	J/mol×K	1237.53	Joback Method
cpg	1174.64	J/mol×K	1276.60	Joback Method
dvisc	0.0001692	Pa×s	633.34	Joback Method

dvisc	0.0000958	Pa×s	701.48	Joback Method
dvisc	0.0000600	Pa×s	769.62	Joback Method
dvisc	0.0000405	Pa×s	837.76	Joback Method
dvisc	0.0000290	Pa×s	905.89	Joback Method
dvisc	0.0000218	Pa×s	974.03	Joback Method
dvisc	0.0000170	Pa×s	1042.17	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=U390379&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