Succinic acid, hept-2-yl 4-chloro-2-methoxyphenyl ester

Inchi: InChI=1S/C18H25ClO5/c1-4-5-6-7-13(2)23-17(20)10-11-18(21)24-15-9-8-14(19)12-16(15

InchiKey: WOWIFMOTLZOFMR-UHFFFAOYSA-N

Formula: C18H25ClO5

SMILES: CCCCCC(C)OC(=O)CCC(=O)Oc1ccc(Cl)cc1OC

Mol. weight [g/mol]: 356.84

Physical Properties

Property code	Value	Unit	Source
gf	-393.38	kJ/mol	Joback Method
hf	-844.10	kJ/mol	Joback Method
hfus	43.08	kJ/mol	Joback Method
hvap	83.98	kJ/mol	Joback Method
log10ws	-5.33		Crippen Method
logp	4.546		Crippen Method
mcvol	273.710	ml/mol	McGowan Method
pc	1480.43	kPa	Joback Method
rinpol	2444.00		NIST Webbook
rinpol	2444.00		NIST Webbook
tb	859.87	K	Joback Method
tc	1067.41	K	Joback Method
tf	525.55	K	Joback Method
vc	1.044	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	815.99	J/mol×K	859.87	Joback Method
cpg	830.06	J/mol×K	894.46	Joback Method
cpg	842.95	J/mol×K	929.05	Joback Method
cpg	854.66	J/mol×K	963.64	Joback Method
cpg	865.20	J/mol×K	998.23	Joback Method
cpg	874.56	J/mol×K	1032.82	Joback Method
cpg	882.74	J/mol×K	1067.41	Joback Method
dvisc	0.0004037	Pa×s	525.55	Joback Method

dvisc	0.0002334	Pa×s	581.27	Joback Method
dvisc	0.0001485	Pa×s	636.99	Joback Method
dvisc	0.0001016	Pa×s	692.71	Joback Method
dvisc	0.0000736	Pa×s	748.43	Joback Method
dvisc	0.0000557	Pa×s	804.15	Joback Method
dvisc	0.0000437	Pa×s	859.87	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390937&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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