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

Inchi: InChI=1S/C18H23ClO5/c1-3-4-5-6-13(2)23-17(21)9-10-18(22)24-16-8-7-15(19)11-14(16)

InchiKey: RDILTAOMOJNJDS-UHFFFAOYSA-N

Formula: C18H23ClO5

SMILES: CCCCCC(C)OC(=O)CCC(=O)Oc1ccc(Cl)cc1C=O

Mol. weight [g/mol]: 354.82

Physical Properties

Property code	Value	Unit	Source
gf	-387.90	kJ/mol	Joback Method
hf	-797.46	kJ/mol	Joback Method
hfus	44.18	kJ/mol	Joback Method
hvap	88.29	kJ/mol	Joback Method
log10ws	-5.45		Crippen Method
logp	4.350		Crippen Method
mcvol	269.410	ml/mol	McGowan Method
pc	1589.81	kPa	Joback Method
rinpol	2519.00		NIST Webbook
rinpol	2519.00		NIST Webbook
tb	886.11	K	Joback Method
tc	1098.02	K	Joback Method
tf	545.32	K	Joback Method
vc	1.044	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	801.07	J/mol×K	886.11	Joback Method
cpg	853.43	J/mol×K	1062.70	Joback Method
cpg	845.15	J/mol×K	1027.39	Joback Method
cpg	835.79	J/mol×K	992.07	Joback Method
cpg	825.33	J/mol×K	956.75	Joback Method
cpg	813.76	J/mol×K	921.43	Joback Method
cpg	860.65	J/mol×K	1098.02	Joback Method
dvisc	0.0000629	Pa×s	886.11	Joback Method

dvisc	0.0000797	Pa×s	829.31	Joback Method
dvisc	0.0001047	Pa×s	772.51	Joback Method
dvisc	0.0001436	Pa×s	715.71	Joback Method
dvisc	0.0002079	Pa×s	658.92	Joback Method
dvisc	0.0003229	Pa×s	602.12	Joback Method
dvisc	0.0005496	Pa×s	545.32	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389918&Units=SI

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