Succinic acid, 3-chlorophenyl 2,4-dimethylpent-3-yl ester

Inchi: InChI=1S/C17H23ClO4/c1-11(2)17(12(3)4)22-16(20)9-8-15(19)21-14-7-5-6-13(18)10-14/

InchiKey: PFIAIOANBDSKKG-UHFFFAOYSA-N

Formula: C17H23ClO4

SMILES: CC(C)C(OC(=O)CCC(=O)Oc1cccc(Cl)c1)C(C)C

Mol. weight [g/mol]: 326.81

Physical Properties

Property code	Value	Unit	Source
gf	-292.05	kJ/mol	Joback Method
hf	-690.33	kJ/mol	Joback Method
hfus	32.64	kJ/mol	Joback Method
hvap	77.91	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	4.249		Crippen Method
mcvol	253.750	ml/mol	McGowan Method
pc	1659.19	kPa	Joback Method
rinpol	2197.00		NIST Webbook
rinpol	2197.00		NIST Webbook
tb	808.71	K	Joback Method
tc	1021.14	K	Joback Method
tf	449.53	K	Joback Method
vc	0.959	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	733.01	J/mol×K	808.71	Joback Method
cpg	747.82	J/mol×K	844.11	Joback Method
cpg	761.49	J/mol×K	879.52	Joback Method
cpg	774.04	J/mol×K	914.92	Joback Method
cpg	785.49	J/mol×K	950.33	Joback Method
cpg	795.86	J/mol×K	985.73	Joback Method
cpg	805.16	J/mol×K	1021.14	Joback Method
dvisc	0.0009960	Pa×s	449.53	Joback Method

dvisc	0.0004649	Pa×s	509.39	Joback Method
dvisc	0.0002547	Pa×s	569.26	Joback Method
dvisc	0.0001565	Pa×s	629.12	Joback Method
dvisc	0.0001046	Pa×s	688.98	Joback Method
dvisc	0.0000746	Pa×s	748.85	Joback Method
dvisc	0.0000559	Pa×s	808.71	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=U390510&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