Succinic acid, 4-chloro-3-methylphenyl 2,4,4-trimethylpentyl ester

Inchi: InChI=1S/C19H27ClO4/c1-13(11-19(3,4)5)12-23-17(21)8-9-18(22)24-15-6-7-16(20)14(2)10-15/h6-7,10,13H,8-9,11-12H2,1-5H3

InchiKey: RXOMKGPKYMBOPH-UHFFFAOYSA-N

Formula: C19H27ClO4

SMILES: Cc1cc(OC(=O)CCC(=O)OCC(C)CC(C)(C)C)ccc1Cl

Mol. weight [g/mol]: 354.87

Physical Properties

Property code	Value	Unit	Source
gf	-277.12	kJ/mol	Joback Method
hf	-741.27	kJ/mol	Joback Method
hfus	37.06	kJ/mol	Joback Method
hvap	82.50	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	4.950		Crippen Method
mcvol	281.930	ml/mol	McGowan Method
pc	1414.37	kPa	Joback Method
rinpol	2363.00		NIST Webbook
rinpol	2363.00		NIST Webbook
tb	857.10	K	Joback Method
tc	1070.03	K	Joback Method
tf	517.01	K	Joback Method
vc	1.071	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	846.94	J/mol×K	857.10	Joback Method
cpg	910.53	J/mol×K	1034.54	Joback Method
cpg	899.97	J/mol×K	999.05	Joback Method
cpg	888.37	J/mol×K	963.56	Joback Method
cpg	875.69	J/mol×K	928.08	Joback Method
cpg	861.89	J/mol×K	892.59	Joback Method
cpg	920.08	J/mol×K	1070.03	Joback Method
dvisc	0.0000399	Pa×s	857.10	Joback Method

dvisc	0.0000520	Pa×s	800.42	Joback Method
dvisc	0.0000706	Pa×s	743.74	Joback Method
dvisc	0.0001009	Pa×s	687.05	Joback Method
dvisc	0.0001537	Pa×s	630.37	Joback Method
dvisc	0.0002545	Pa×s	573.69	Joback Method
dvisc	0.0004705	Pa×s	517.01	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=U389548&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