Sebacic acid, 4-chlorophenyl isobutyl ester

Inchi: InChI=1S/C20H29ClO4/c1-16(2)15-24-19(22)9-7-5-3-4-6-8-10-20(23)25-18-13-11-17(21)
InchiKey: STWAQESNFGZCHB-UHFFFAOYSA-N
Formula: C20H29ClO4
SMILES: CC(C)COC(=O)CCCCCCCCC(=O)Oc1ccc(Cl)cc1
Mol. weight [g/mol]: 368.89

Physical Properties

Property code	Value	Unit	Source
gf	-261.91	kJ/mol	Joback Method
hf	-741.69	kJ/mol	Joback Method
hfus	47.46	kJ/mol	Joback Method
hvap	85.36	kJ/mol	Joback Method
log10ws	-6.11		Crippen Method
logp	5.565		Crippen Method
mcvol	296.020	ml/mol	McGowan Method
pc	1313.70	kPa	Joback Method
rinpol	2715.00		NIST Webbook
rinpol	2715.00		NIST Webbook
tb	878.23	K	Joback Method
tc	1085.09	K	Joback Method
tf	513.34	K	Joback Method
vc	1.139	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	905.47	J/mol×K	878.23	Joback Method
cpg	920.52	J/mol×K	912.71	Joback Method
cpg	934.40	J/mol×K	947.18	Joback Method
cpg	947.12	J/mol×K	981.66	Joback Method
cpg	958.72	J/mol×K	1016.14	Joback Method
cpg	969.21	J/mol×K	1050.62	Joback Method
cpg	978.64	J/mol×K	1085.09	Joback Method
dvisc	0.0005407	Pa×s	513.34	Joback Method

dvisc	0.0002839	Pa×s	574.15	Joback Method
dvisc	0.0001687	Pa×s	634.97	Joback Method
dvisc	0.0001098	Pa×s	695.78	Joback Method
dvisc	0.0000765	Pa×s	756.60	Joback Method
dvisc	0.0000563	Pa×s	817.41	Joback Method
dvisc	0.0000432	Pa×s	878.23	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=U354813&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