Pimelic acid, butyl 3-chlorophenyl ester

Inchi: InChI=1S/C17H23ClO4/c1-2-3-12-21-16(19)10-5-4-6-11-17(20)22-15-9-7-8-14(18)13-15/
InchiKey: QOMQERLVGRWLPX-UHFFFAOYSA-N
Formula: C17H23ClO4
SMILES: CCCCOC(=O)CCCCCC(=O)Oc1cccc(Cl)c1
Mol. weight [g/mol]: 326.81

Physical Properties

Property code	Value	Unit	Source
gf	-284.73	kJ/mol	Joback Method
hf	-674.49	kJ/mol	Joback Method
hfus	43.21	kJ/mol	Joback Method
hvap	79.07	kJ/mol	Joback Method
log10ws	-5.10		Crippen Method
logp	4.539		Crippen Method
mcvol	253.750	ml/mol	McGowan Method
pc	1627.22	kPa	Joback Method
rinpol	2412.00		NIST Webbook
rinpol	2412.00		NIST Webbook
tb	810.03	K	Joback Method
tc	1014.58	K	Joback Method
tf	494.53	K	Joback Method
vc	0.977	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	731.34	J/mol×K	810.03	Joback Method
cpg	792.66	J/mol×K	980.49	Joback Method
cpg	782.38	J/mol×K	946.39	Joback Method
cpg	771.12	J/mol×K	912.30	Joback Method
cpg	758.88	J/mol×K	878.21	Joback Method
cpg	745.62	J/mol×K	844.12	Joback Method
cpg	801.99	J/mol×K	1014.58	Joback Method
dvisc	0.0000722	Pa×s	810.03	Joback Method

dvisc	0.0000918	Pa×s	757.45	Joback Method
dvisc	0.0001210	Pa×s	704.86	Joback Method
dvisc	0.0001667	Pa×s	652.28	Joback Method
dvisc	0.0002430	Pa×s	599.70	Joback Method
dvisc	0.0003807	Pa×s	547.11	Joback Method
dvisc	0.0006561	Pa×s	494.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416670&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