Pimelic acid, 4-chlorobenzyl isobutyl ester

Inchi: InChI=1S/C18H25ClO4/c1-14(2)12-22-17(20)6-4-3-5-7-18(21)23-13-15-8-10-16(19)11-9-

InchiKey: JWSCNJHYHPYEMX-UHFFFAOYSA-N

Formula: C18H25ClO4

SMILES: CC(C)COC(=O)CCCCCC(=O)OCc1ccc(Cl)cc1

Mol. weight [g/mol]: 340.84

Physical Properties

Property code	Value	Unit	Source
gf	-278.75	kJ/mol	Joback Method
hf	-700.41	kJ/mol	Joback Method
hfus	42.28	kJ/mol	Joback Method
hvap	80.91	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	4.533		Crippen Method
mcvol	267.840	ml/mol	McGowan Method
pc	1517.57	kPa	Joback Method
rinpol	2415.00		NIST Webbook
rinpol	2415.00		NIST Webbook
tb	832.47	K	Joback Method
tc	1038.76	K	Joback Method
tf	490.80	K	Joback Method
vc	1.026	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	788.94	J/mol×K	832.47	Joback Method
cpg	803.61	J/mol×K	866.85	Joback Method
cpg	817.18	J/mol×K	901.23	Joback Method
cpg	829.67	J/mol×K	935.62	Joback Method
cpg	841.11	J/mol×K	970.00	Joback Method
cpg	851.52	J/mol×K	1004.38	Joback Method
cpg	860.90	J/mol×K	1038.76	Joback Method
dvisc	0.0006700	Pa×s	490.80	Joback Method

dvisc	0.0003599	Pa×s	547.75	Joback Method
dvisc	0.0002174	Pa×s	604.69	Joback Method
dvisc	0.0001432	Pa×s	661.63	Joback Method
dvisc	0.0001008	Pa×s	718.58	Joback Method
dvisc	0.0000747	Pa×s	775.52	Joback Method
dvisc	0.0000577	Pa×s	832.47	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=U406793&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